EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
S1	2	("20050272930").PN.	US-PGPUB; USPAT; DERWENT	OR	OFF	2007/04/18 16:20
S2	2	("6984738").PN.	US-PGPUB; USPAT; DERWENT	OR	OFF	2007/04/18 15:28
S3	315	(549/6).CCLS.	US-PGPUB; USPAT; DERWENT	OR	OFF	2007/04/18 16:32
S4	431	(549/75).CCLS.	US-PGPUB; USPAT; DERWENT	OR	OFF	2007/04/19 12:50
S5	357	(549/497).CCLS.	US-PGPUB; USPAT; DERWENT	OR	OFF	2007/04/19 12:50

25/04/2007,10569824IIa.trn

Connecting via Winsock to STN

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LOGINID:SSPTASXY1626

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'HCAPLUS' AT 13:48:43 ON 18 APR 2007
FILE 'HCAPLUS' ENTERED AT 13:48:43 ON 18 APR 2007
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	60.57	232.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.58	-8.58

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	60.57	232.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.58	-8.58

FILE 'REGISTRY' ENTERED AT 13:48:53 ON 18 APR 2007
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STRUCTURE FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9
DICTIONARY FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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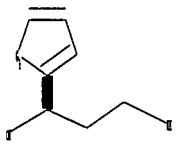
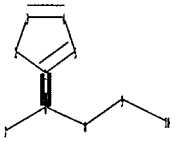
Uploading C:\Program Files\Stnexp\Queries\10569824IIa.str





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6 7 8 9 10
ring nodes :
1 2 3 4 5
chain bonds :
1-6 6-7 6-8 8-9 9-10
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-6 2-3 3-4 4-5 6-7 6-8 8-9 9-10

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L5 STRUCTURE UPLOADED

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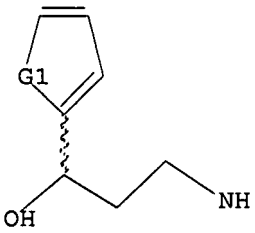
L5 HAS NO ANSWERS
L5 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -      418 TO ITERATE

100.0% PROCESSED      418 ITERATIONS                          12 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         7134 TO     9586
PROJECTED ANSWERS:              33 TO      447

L6            12 SEA SSS SAM L5

=> s l5 full
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FULL SCREEN SEARCH COMPLETED -     8529 TO ITERATE

100.0% PROCESSED     8529 ITERATIONS                        245 ANSWERS
SEARCH TIME: 00.00.01

L7           245 SEA SSS FUL L5

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                             172.10     404.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                               0.00      -8.58

FILE 'HCAPLUS' ENTERED AT 13:49:33 ON 18 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 18 Apr 2007 VOL 146 ISS 17
FILE LAST UPDATED: 16 Apr 2007 (20070416/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7
L8 126 L7

=> d ed abs ibib hitstr 1-126

L8 ANSWER 1 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Mar 2007
AB The present invention concerns Candida dehydrogenases for the reduction of substituted alkanols, such as 3-methylamino-1-(2-thienyl)-propane-1-one. The invention concerns further nucleic acids, which code for these proteins, nucleic acid constructs, vectors, genetically altered microorganisms as well as procedures for production of optically active substituted alkanols, such as (S)-3-methylamino-1-(2-thienyl)-(S)-propanol.
ACCESSION NUMBER: 2007:329401 HCAPLUS
DOCUMENT NUMBER: 146:311480
TITLE: Candida dehydrogenases and their use in production of optically active alkanols
INVENTOR(S): Breuer, Michael; Friedrich, Thomas; Kesseler, Maria
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 18pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 102005044736	A1	20070322	DE 2005-102005044736	20050919
WO 2007033928	A1	20070329	WO 2006-EP66336	20060914

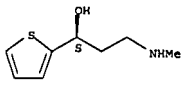
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: DE 2005-102005044736A 20050919

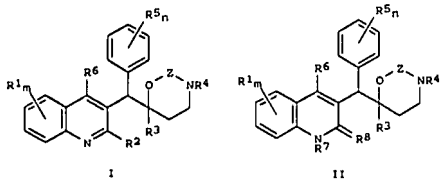
OTHER SOURCE(S): CASREACT 146:311480
IT 116539-55-0P
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(Candida dehydrogenases and their use in production of optically active alkanols)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

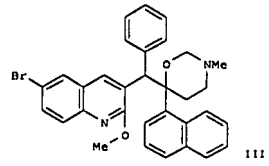
Absolute stereochemistry. Rotation (-).

L8 ANSWER 1 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 2 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 09 Feb 2007
GI





AB Use of a compound for the manufacture of a medicament for the treatment of a bacterial infection provided that the bacterial infection is other than a Mycobacterial infection, said compound being a compound of formula I & II [R1 = H, halo(alkyl), cyano, etc.; R2 = H, halo, mercapto, etc.; R3 = alkyl, (un)substituted aryl(alkyl) or heterocyclyl(alkyl); R4 = H, alkyl or benzyl; R5 = H, halo(alkyl), (aryl)alkyl, etc.; R6 = H, alkyl, (un)substituted aryl or heterocyclyl; R7 = H or alkyl; R8 = oxo; Z = CH2 or C=O; m = 1-4; n = 1-5], a pharmaceutically acceptable acid or base addition salt, a quaternary amine, a stereochem. isomeric form, a tautomeric form or a N-oxide form thereof. For example, III was provided in a multi-step synthesis starting from the reaction of benzenepropanoyl chloride with 4-bromobenzenamine. I showed antibacterial activity in Microtitre plate assay.
ACCESSION NUMBER: 2007:150180 HCAPLUS
DOCUMENT NUMBER: 146:229198
TITLE: Preparation of quinoline derivatives as antibacterial agents
INVENTOR(S): Andries, Koenraad Jozef Lodewijk Marcel; Koul, Anil; Guillemont, Jerome Emile Georges; Pasquier, Elisabeth Therese Jeanne
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 63pp.
CODEN: PIXXD2

L8 ANSWER 2 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

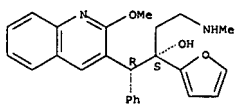
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007014934	A2	20070208	WO 2006-EP64847	20060731

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: EP 2005-107155 A 20050803

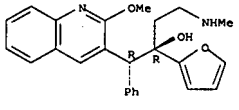
OTHER SOURCE(S): MARPAT 146:229198
IT 861709-49-1P 861709-51-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinoline derivs. as antibacterial agents)
RN 861709-49-1 HCAPLUS
CN 3-Quinolineethanol, α-2-furanyl-2-methoxy-α-[2-(methylamino)ethyl]-β-phenyl-, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



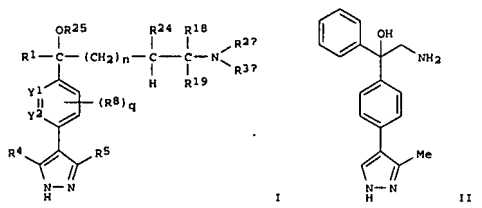
RN 861709-51-5 HCAPLUS
CN 3-Quinolineethanol, α-2-furanyl-2-methoxy-α-[2-(methylamino)ethyl]-β-phenyl-, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L8 ANSWER 2 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L8 ANSWER 3 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Dec 2006
GI



I II

AB The invention provides a compound of the formula I or a salt, solvate, tautomer or N-oxide thereof; wherein n = 0 or 1; Y1 and Y2 = CH, IR8 and N; q = 0-2; R1 = an aryl or heteroaryl group of 5 to 10 ring members; R2a and R3a = H, (un)substituted C1-4 hydrocarbyl or (un)substituted C1-4 acyl; or NR2aR3a forms an imidazole or 4-7 membered heterocyclic ; R18, R19 = H or Me; R24 = H or is part of a heterocyclic ring with R2a; R25 = H
or (un)substituted C1-4 alkyl group ; R4 and R5 = H, halo, etc.; and R8 = OH, halo, etc. I have PKA or PKB inhibiting or modulating activity and can be used to treat conditions mediated by these 2 enzymes. A process for preparing I is also claimed. For example, II was prepared by reacting
2-(4-chlorophenyl)-2-(4-iodophenyl)oxirane with ammonia to form an amine which was reacted with 3-methyl-1-sulfonic acid dimethylamide-pyrazole boronic acid; subsequent removal of the dimethylaminosulfonyl group from the intermediate formed gave II. In in vitro assays, II had IC50's of <1 μM against PKB and PKA activity.

ACCESSION NUMBER: 2006:1356561 HCAPLUS
DOCUMENT NUMBER: 146:100678
TITLE: Preparation of pyrazole containing aryl-alkylamines and heteroaryl-alkylamines as protein kinase inhibitors
INVENTOR(S): Woodhead, Steven John; Downham, Robert; Hamlett, Christopher; Howard, Steven; Sore, Hannah Fiona; Verdonk, Marinus Leendert; Walker, David Winter; Luke, Richard William Arthur
PATENT ASSIGNEE(S): Astex Therapeutics Limited, UK; The Institute of Cancer ResearchRoyal Cancer Hospital; Cancer Research Technology Limited; Astrazeneca AB
SOURCE: PCT Int. Appl., 250pp.
CODEN: PIXXD2

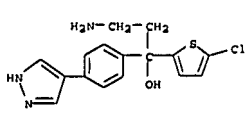
L8 ANSWER 3 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006136830	A1	20061228	WO 2006-GB2287	20060621

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

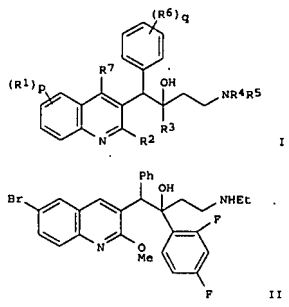
PRIORITY APPLN. INFO.: GB 2005-12642 A 20050621
US 2005-692482P P 20050621
US 2006-744141P P 20060403

OTHER SOURCE(S): MARPAT 146:100678
IT 917900-06-2P, 3-Amino-1-(5-chlorothiophen-2-yl)-1-[4-(1H-pyrazol-4-yl)phenyl]propan-1-ol
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrazole containing aryl-alkylamines and heteroaryl-alkylamines as protein kinase inhibitors)
RN 917900-06-2 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-chloro-α-[4-(1H-pyrazol-4-yl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 4 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 15 Dec 2006
GI



I

II

AB Use of title compds. (I; R1 = H, halo, polyhaloalkyl, alkyl, hydroxyalkyl, alkoxy, Ar, Het; p, q = 1, 2; R2 = alkoxy, alkoxyalkoxy, alkylthio; R3 = alkyl, Ar, Het, Het1; R4, R5 = H, alkyl, benzyl; R4R5N = (substituted) pyrrolidinyl, pyrrolinyl, pyrrolyl, imidazolidinyl, pyrazolidinyl, imidazolinyl, pyrazolinyl, imidazolyl, pyrazolyl, triazolyl, piperidinyl, pyridinyl, piperazinyl, pyridazinyl, pyrimidinyl, pyrazinyl, triazinyl, morpholinyl, thiomorpholinyl; R6 = H, halo, polyhaloalkyl, alkyl, alkoxy, alkylthio; 2 vicinal R6 may = CH:CHCH:CH; R7 = H, alkyl, Ar, Het, Het1; Ar = (substituted) Ph, naphthyl, acenaphthyl, 1,2-dihydroacenaphthyl, tetrahydronaphthyl; Het = (substituted) piperidyl, pyrrolyl, N-phenoxypiperidyl, pyrazolyl, triazolyl, imidazolyl, furyl, pyridyl, pyrimidyl, pyrazinyl, etc.; Het1 = (substituted) quinolyl, quinoxalinyl, indolyl, benzimidazolyl, benzofuryl, benzothienyl, 2,3-dihydrobenzodioxinyl, etc.; with provisos], for manufacture of a medicament for
treatment of bacterial infection is claimed. Thus, a diastereomer of title compound (II) (preparation outlined) showed an IC90 = 10.8 μg/mL against
Streptococcus mutans ATCC33402.

ACCESSION NUMBER: 2006:1311179 HCAPLUS
DOCUMENT NUMBER: 146:62607
TITLE: Preparation of aminohydroxyphenylbutylquinolines as antibacterials.
INVENTOR(S): Andries, Koenraad Jozef Lodewijk Marcel; Koul, Anil; Guillemont, Jerome Emile Georges; Pasquier, Elisabeth Therese Jeanne; Lancois, David Francis Alain
PATENT ASSIGNEE(S): Janssen Pharmaceutica N. V., Belg.

L8 ANSWER 4 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
SOURCE: PCT Int. Appl., 63pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006131519	A1	20061214	WO 2006-EP62934	20060606
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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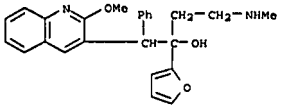
JP 2006342109	A	20061221	JP 2005-169982	20050609
CA 2528849	A1	20061208	CA 2005-2528849	20051206
EE 200500034	A	20070215	EE 2005-34	20051206
AU 2005242142	A1	20070104	AU 2005-242142	20051207
US 2006281741	A1	20061214	US 2005-296918	20051208
TR 200504891	A2	20070122	TR 2005-4891	20051208
BR 2005006121	A	20070213	BR 2005-6121	20051208
PRIORITY APPLN. INFO.:			EP 2005-105023 A	20050608
			US 2005-296918 A	20051208

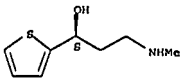
OTHER SOURCE(S): MARPAT 146:62607
IT 916800-59-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of aminohydroxyphenylbutylquinolines as antibacterials)
RN 916800-59-4 HCAPLUS
CN 3-Quinolineethanol, α-2-furanyl-2-methoxy-α-[2-(methylamino)ethyl]-β-phenyl- (CA INDEX NAME)



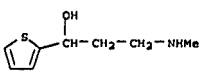
L8 ANSWER 4 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Nov 2006
AB The synthesis of 5-phenylthio-1,3-oxazin-4-ones, through a hetero Diels-Alder strategy, is described. The cycloadducts thus prepared are useful intermediates for the synthesis of 1,3-amino alcs., valuable intermediates in the preparation of biol. significant mols., e.g., optically active Duloxetines and Fluoxetines. In the course of this elaboration a novel microwave assisted desulfurization reaction is reported.
ACCESSION NUMBER: 2006:1245399 HCAPLUS
DOCUMENT NUMBER: 146:142584
TITLE: 5-Phenylthio-1,3-oxazinan-4-ones via hetero Diels-Alder reactions: synthesis of (R)- and (S)-Duloxetines and Fluoxetines
AUTHOR(S): Panunzio, Mauro; Tamanini, Emiliano; Bandini, Elisa; Campana, Eileen; D'Aurizio, Antonio; Vicennati, Paola
CORPORATE SOURCE: I.S.O.F-C.N.R. Department of Chemistry, University of Bologna, G. Ciamician, Bologna, 40126, Italy
SOURCE: Tetrahedron (2006), 62(52), 12270-12280
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 116539-55-0P 116539-56-1P 116539-57-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 5-phenylthio-tetrahydro-1,3-oxazin-4-ones via hetero Diels-Alder reactions as intermediates for (R)- and (S)-Duloxetines and Fluoxetines)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



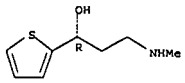
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

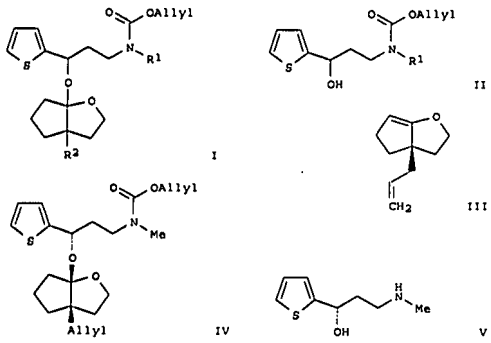
Absolute stereochemistry. Rotation (+).

L8 ANSWER 5 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 05 Oct 2006
GI



AB Disclosed is a method for the preparation of 1-(2-thienyl)-3-(alkylamino)propanols, via alcoholysis of I [R1 = alkyl, R2 = (un)substituted alkyl, alkenyl, aryl or aralkyl] followed by reduction or hydrolysis of the resultant II [R1 = alkyl]. For instance, successive Mannich reaction of 2-acetylthiophene with paraformaldehyde and benzylamine hydrochloride (86% yield), debenzylation/N-acylation with allyl chloroformate (91% yield), and selective reduction of the keto (75% yield) gave racemic alc. II (R1 = Me). Treatment of this alc. with chiral bicyclooctene III led to ketal IV and its diastereomer (total 96.7% yield). IV underwent deacetalization with methanol in the presence of PTS·H2O to afford (S)-II (R1 = Me) (90% yield), which was either deprotected with Pd(OAc)2/PPh3 (29.8% yield, >99.5% ee) or hydrolyzed with NaOH (45.0% yield, >99.5% ee) to give chiral alc. V. The diastereomer of IV can be reused by conversion into its racemate II (R1 = Me) with dilute HCl. The invented process features high yield and high purity.

ACCESSION NUMBER: 2006:1031462 HCAPLUS
DOCUMENT NUMBER: 145:397355
TITLE: Process for the preparation of 1-(2-thienyl)-3-alkylaminopropanols
INVENTOR(S): Yamada, Toshirou; Sakamoto, Kei; Watanabe, Kazunori; Nakano, Yasushi

L8 ANSWER 6 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
PATENT ASSIGNEE(S): Zeon Corporation, Japan
SOURCE: PCT Int. Appl., 27pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

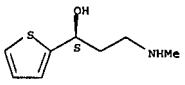
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006104249	A1	20061005	WO 2006-JP307162	20060329

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: JP 2005-95277 A 20050329

OTHER SOURCE(S): MARPAT 145:397355
IT 116539-55-0P
RL: IMP (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of methylaminoethyl thiophenemethanol)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

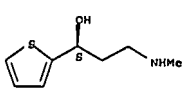


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 15 Sep 2006
AB (±)-3-(N,N-Dimethylamino)-1-(2-thienyl)propan-1-ol (I), prepared from 2-acetylthiophene in a two-step overall yield of 79%, is resolved into (S)-I of 93% ee as its diastereomeric salt (II) with (S)-mandelic acid according to Eli Lilly's procedures developed for the resolution-racemization-recycle (RRR) synthesis of duloxetine (III) with some modifications in terms of practicality. On its liberation from II, (S)-I undergoes N-demethylative Et carbamate formation in two discrete but successive steps in an overall yield of 87% from II: (1) O-Et carbonate formation and (2) Et carbamate formation with concomitant loss of the N-Me group. Alkaline hydrolysis then affords (S)-3-(N-methylamino)-1-(2-thienyl)propan-1-ol of 100% ee, an alleged penultimate precursor to duloxetine, in 75% yield after a single recrystn. from ethylcyclohexane. In the overall process thus developed, PhMe is substituted successfully for Me3COMe, a solvent that has been used favorably in Eli Lilly's original RRR synthesis of III.

ACCESSION NUMBER: 2006:948585 HCAPLUS
DOCUMENT NUMBER: 145:454890
TITLE: Synthesis of (S)-3-(N-Methylamino)-1-(2-thienyl)propan-1-ol: Revisiting Eli Lilly's Resolution-Racemization-Recycle Synthesis of Duloxetine for Its Robust Processes
AUTHOR(S): Fujima, Yoshito; Ikunaka, Masaya; Inoue, Toru; Matsumoto, Jun
CORPORATE SOURCE: Research Development Center, Nagase Co. Ltd., Nishi-ku, Kobe, 651-2241, Japan
SOURCE: Organic Process Research & Development (2006), 10(5), 905-913
CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 116539-55-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (S)-3-(N-methylamino)-1-(2-thienyl)propan-1-ol, an intermediate for duloxetine)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

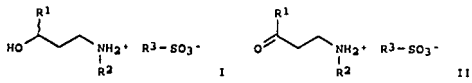
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L8 ANSWER 8 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 28 Aug 2006
GI



AB Provided is a process for the preparation of N-monosubstituted β-aminoalc.
sulfonates of formula I. Compds. of formula I wherein R1 is (un)substituted C6-20 aryl or (un)substituted C4-12 heteroaryl; R2 is C1-4-alkyl or (un)substituted C6-20 aryl; R3 is selected from the group consisting of C1-18 alkyl, C6-20 cycloalkyl, C6-20 aryl and C7-20 aralkyl residues, and the process for preparing compds. of formula I are claimed. The process comprising the steps of a) reacting a Me ketone, a primary amine, formaldehyde and a sulfonic acid, at a pressure above 1.5 bar, optionally in a organic solvent, said organic solvent optionally containing water,
to afford N-monosubstituted β-amino ketone sulfonates of formula II, wherein R1, R2 and R3 are as defined above, and b) asym. hydrogenating said sulfonates in the presence of a base and a catalyst, comprising a transition metal and a diphosphine ligand, in a polar solvent, optionally in the presence of water.

ACCESSION NUMBER: 2006:866581 HCAPLUS
DOCUMENT NUMBER: 145:271387
TITLE: Process for the preparation of enantiomerically pure 1-substituted-3-amino alcohols using methyl ketones, primary amines, formaldehydes and sulfonic acids
INVENTOR(S): Brieden, Walter; Clausen, Martin; McGarrity, John; Mettler, Hanspeter; Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 38pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006087166	A1	20060824	WO 2006-EP1334	20060214

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,

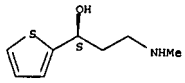
L8 ANSWER 8 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
EP 1693371 A1 20060823 EP 2005-3657 20050221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU
PRIORITY APPLN. INFO.: EP 2005-3657 A 20050221

OTHER SOURCE(S): CASREACT 145:271387; MARPAT 145:271387
IT 863094-27-3P 906812-56-4P 906812-57-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(product; preparation of enantiomerically pure sulfonate salts of substituted amino alcs. and amino ketones by reacting Me ketones, primary amine, formaldehyde and sulfonic acids)
RN 863094-27-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-, 4-methylbenzenesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

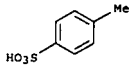
CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).



CM 2

CRN 104-15-4
CMF C7 H8 O3 S



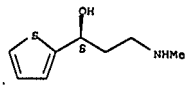
RN 906812-56-4 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-, methanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0

L8 ANSWER 8 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).



CM 2

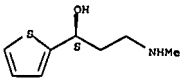
CRN 75-75-2
CMF C H4 O3 S

RN 906812-57-5 HCAPLUS
CN Bicyclo[2.2.1]heptane-1-methanesulfonic acid, 7,7-dimethyl-2-oxo-, (1S,4R)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).

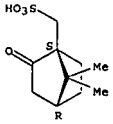


CM 2

CRN 3144-16-9
CMF C10 H16 O4 S

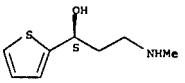
Absolute stereochemistry. Rotation (+).

L8 ANSWER 8 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



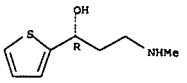
IT 116539-55-0 116539-57-2 863094-39-7
863094-46-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of enantiomerically pure sulfonate salts of
substituted amino alcs. and amino ketones by reacting Me ketones, primary amine, formaldehyde and sulfonic acids)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

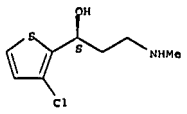
Absolute stereochemistry. Rotation (+).



RN 863094-39-7 HCAPLUS
CN 2-Thiophenemethanol, 3-chloro-α-[2-(methylamino)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

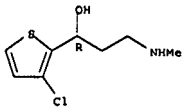
Absolute stereochemistry. Rotation (-).

L8 ANSWER 8 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 863094-46-6 HCAPLUS
CN 2-Thiophenemethanol, 3-chloro-α-[2-(methylamino)ethyl]-, (αR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

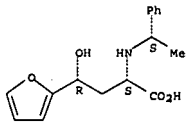


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L8 ANSWER 9 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 26 Jul 2006
AB A new synthesis of enantiomerically highly enriched N-substituted furoylalanines has been developed. This process involves the combination of crystallization induced asym. transformation (CIAT) and a conjugate addition of N-nucleophiles to furoylacrylic acids. Further transformations to furoylalanines and substituted furylcarbinols are also described.
ACCESSION NUMBER: 2006:725707 HCAPLUS
DOCUMENT NUMBER: 145:336293
TITLE: Crystallisation induced asymmetric transformation (CIAT) in the synthesis of furoylalanines and furylcarbinols
AUTHOR(S): Jakubec, Pavol; Berkes, Dusan; Siska, Richard; Gardianova, Maria; Povazanec, Frantisek
CORPORATE SOURCE: Department of Organic Chemistry, Slovak University of Technology, Bratislava, SK-812 37, Slovakia
SOURCE: Tetrahedron: Asymmetry (2006), 17(11), 1629-1637 CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:336293
IT 909804-91-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of furoylalanines and furylcarbinols via crystallization-induced asym. transformation and conjugate addition of N-nucleophiles to furoylacrylic acids)
RN 909804-91-7 HCAPLUS
CN 2-Furanbutanoic acid, γ-hydroxy-α-[[(1S)-1-phenylethyl]amino]-, (αS,γR)- (9CI) (CA INDEX NAME)

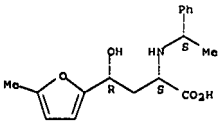
Absolute stereochemistry. Rotation (-).



IT 909804-92-8P 909804-93-9P 909804-94-0P
909804-95-1P 909804-96-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of furoylalanines and furylcarbinols via crystallization-induced asym. transformation and conjugate addition of N-nucleophiles to furoylacrylic acids)

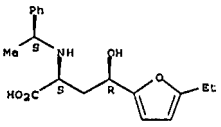
L8 ANSWER 9 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 909804-92-8 HCAPLUS
CN 2-Furanbutanoic acid, γ-hydroxy-5-methyl-α-[[(1S)-1-phenylethyl]amino]-, (αS,γR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



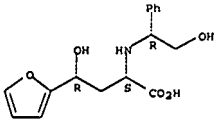
RN 909804-93-9 HCAPLUS
CN 2-Furanbutanoic acid, 5-ethyl-γ-hydroxy-α-[[(1S)-1-phenylethyl]amino]-, (αS,γR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 909804-94-0 HCAPLUS
CN 2-Furanbutanoic acid, γ-hydroxy-α-[[(1R)-2-hydroxy-1-phenylethyl]amino]-, (αS,γR)- (9CI) (CA INDEX NAME)

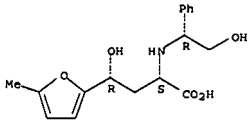
Absolute stereochemistry. Rotation (-).



RN 909804-95-1 HCAPLUS
CN 2-Furanbutanoic acid, γ-hydroxy-α-[[(1R)-2-hydroxy-1-phenylethyl]amino]-5-methyl-, (αS,γR)- (9CI) (CA INDEX NAME)

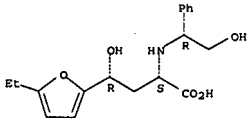
Absolute stereochemistry. Rotation (-).

L8 ANSWER 9 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 909804-96-2 HCAPLUS
CN 2-Furanbutanoic acid, 5-ethyl-γ-hydroxy-α-[[(1R)-2-hydroxy-1-phenylethyl]amino]-, (αS,γR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L8 ANSWER 10 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 14 Jul 2006
AB A mol. distillation process for the purification of (1S)-3-methylamino-1-(2-thienyl)-1-propanol(I) is described in which a mixture containing 25-99% I is distilled in a mol. distillation apparatus
ACCESSION NUMBER: 2006:679804 HCAPLUS
DOCUMENT NUMBER: 145:124444
TITLE: Molecular distillation process for the purification of (1S)-3-methylamino-1-(2-thienyl)-1-propanol
INVENTOR(S): Stuermer, Rainer; Daeuwel, Juergen; Kesseler, Maria; Achatz, Brigitte; Breuer, Michael
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 3 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 102005000867	A1	20060713	DE 2005-102005000867	20050105
WO 2006072465	A1	20060713	WO 2005-EP14161	20051231

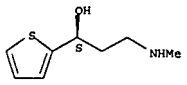
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: DE 2005-102005000867A 20050105

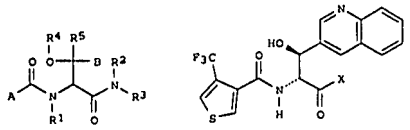
IT 116539-55-0P
RL: PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PYP (Physical process); PREP (Preparation); PROC (Process)
(mol. distillation process for the purification of (1S)-3-methylamino-1-(2-thienyl)-1-propanol)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 10 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 11 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 24 Mar 2006
GI



I II

AB Title compds. I [A = 5 or 6-membered heteroaryl with provisos; B = mono or bicyclic heteroaryl with provisos; R1,R2 = H OH, alkoxy; R3 = alkyl, cyanoalkyl, haloalkyl; R4 = H, alkyl, cycloalkyl, etc.; R5 = H, alkyl] were prepared For example, N-acylation of methylamine with serine ester II (X = OEt) afforded serine amide II (X = NHMe) in 88% yield. Compds. I exhibited very good herbicidal activity against amaranthus retroflexus, i.e., pig weed.
ACCESSION NUMBER: 2006:272514 HCAPLUS
DOCUMENT NUMBER: 144:331692
TITLE: Preparation of heteroaroylserine amides as herbicides
INVENTOR(S): Witschel, Matthias; Stelzer, Frank; Kuehn, Toralf; Parra Rapado, Liliana; Rack, Michael; Hupe, Eike; Zagar, Cyrill; Reinhard, Robert; Sievernich, Bernd; Ehrhardt, Thomas
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

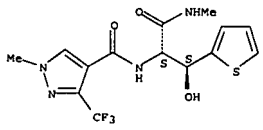
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006029829	A1	20060323	WO 2005-EP9856	20050914

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NO, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: DE 2004-102004045298A 20040916

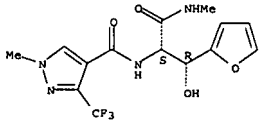
L8 ANSWER 11 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 144:331692
IT 880478-11-5P 880478-27-3P 880478-30-8P 880478-32-0P 880478-33-1P 880478-62-6P 880478-63-7P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaroylserine amides as herbicides)
RN 880478-11-5 HCAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[(1R,2R)-2-hydroxy-1-[(methylamino)carbonyl]-2-(2-thienyl)ethyl]-1-methyl-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 880478-27-3 HCAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[(1R,2S)-2-(2-furanyl)-2-hydroxy-1-[(methylamino)carbonyl]ethyl]-1-methyl-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

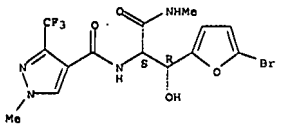
Relative stereochemistry.



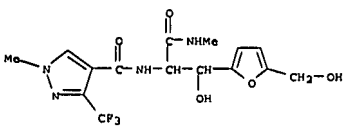
RN 880478-30-8 HCAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[(1R,2S)-2-(5-bromo-2-furanyl)-2-hydroxy-1-[(methylamino)carbonyl]ethyl]-1-methyl-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 11 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

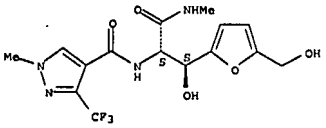


RN 880478-32-0 HCAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-hydroxy-2-[5-(hydroxymethyl)-2-furanyl]-1-[(methylamino)carbonyl]ethyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 880478-33-1 HCAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[(1R,2R)-2-hydroxy-2-[5-(hydroxymethyl)-2-furanyl]-1-[(methylamino)carbonyl]ethyl]-1-methyl-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

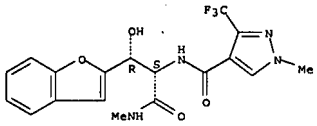
Relative stereochemistry.



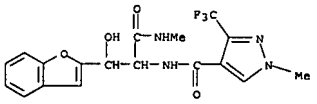
RN 880478-62-6 HCAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[(1R,2S)-2-(2-benzofuranyl)-2-hydroxy-1-[(methylamino)carbonyl]ethyl]-1-methyl-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 11 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

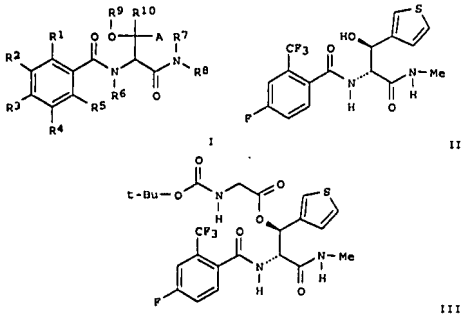


RN 880478-63-7 HCAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[2-(2-benzofuranyl)-2-hydroxy-1-[(methylamino)carbonyl]ethyl]-1-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Mar 2006
GI



I II III

AB Title compds. I [A = mono or bicyclic heteroaryl with provisos; R1 = halo, CN, alkyl, etc.; R2, R3, R4, R5 = H, halo, CN, etc.; R6, R7 = H, OH, alkoxy, etc.; R8 = alkyl, cyanoalkyl, haloalkyl; R9 = H, alkyl, cycloalkyl, etc.; R10 = H, alkyl] were prepared For example, O-acylation of serine II with N-Boc-glycine afforded threo-benzamide III in 24% yield. Compds. I exhibited very good herbicidal activity against amaranthus retroflexus, i.e., pig weed.

ACCESSION NUMBER: 2006:269897 HCAPLUS
DOCUMENT NUMBER: 144:331133
TITLE: Preparation of N-benzoylserine amides as agrochemical herbicides
INVENTOR(S): Witschel, Matthias; Stelzer, Frank; Kuehn, Toralf; Parra Rapado, Liliana; Hupe, Eike; Zagar, Cyrill; Reinhard, Robert; Sievernich, Bernd; Ehrhardt, Thomas
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006029828	A1	20060323	WO 2005-EP9855	20050914

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,

L8 ANSWER 12 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

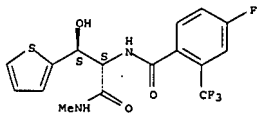
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: DE 2004-102004045300A 20040916

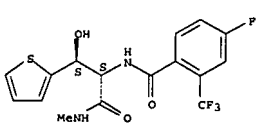
OTHER SOURCE(S): MARPAT 144:331133
IT 880483-76-1P 880484-01-5P 880484-02-6P 880484-03-7P 880484-04-8P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of N-benzoylserine amides as agrochem. herbicides)
RN 880483-76-1 HCAPLUS
CN 2-Thiophenepropanamide, α-[[4-fluoro-2-(trifluoromethyl)benzoyl]amino]-β-hydroxy-N-methyl-, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



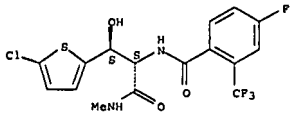
RN 880484-01-5 HCAPLUS
CN 2-Thiophenepropanamide, α-[[4-fluoro-2-(trifluoromethyl)benzoyl]amino]-β-hydroxy-N-methyl-, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



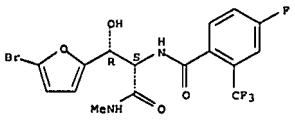
RN 880484-02-6 HCAPLUS
CN 2-Thiophenepropanamide, 5-chloro-α-[[4-fluoro-2-(trifluoromethyl)benzoyl]amino]-β-hydroxy-N-methyl-, (αS,βS)- (9CI) (CA INDEX NAME)

L8 ANSWER 12 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.

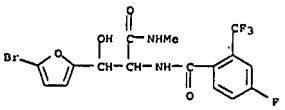


RN 880484-03-7 HCAPLUS
CN 2-Furanpropanamide, 5-bromo-α-[[4-fluoro-2-(trifluoromethyl)benzoyl]amino]-β-hydroxy-N-methyl-, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 880484-04-8 HCAPLUS
CN 2-Furanpropanamide, 5-bromo-α-[[4-fluoro-2-(trifluoromethyl)benzoyl]amino]-β-hydroxy-N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 13 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 27 Jan 2006
AB Ar2CH2XCH2CR1Ar1CH2(CH2)nNR2R3 (Ar1 = (substituted) Ph, naphthalenyl, thienyl; Ar2 = (substituted) Ph; R1 = H, OH, alkyl, alkoxy; R2, R3, R4 = H, alkyl; X = O, S, NR4; n = 0, 1], were prepared Thus, Me2NH and 2-[[3,5-bis(trifluoromethyl)benzyloxy]methyl]-2-phenyloxirane (preparation given) were microwaved in MeOH at 120° for 10 min to give 1-[3,5-bis(trifluoromethyl)benzyloxy]-3-dimethylamino-2-phenylpropan-1-ol isolated as the trifluoroacetate salt. The latter and other title compds. showed IC50 values of 1-100 nM in an NK-1 binding assay.
ACCESSION NUMBER: 2006:79128 HCAPLUS
DOCUMENT NUMBER: 144:170779
TITLE: Preparation of benzyloxyalkylamines as neurokinin-1/selective serotonin reuptake inhibitors (NK1/SSRI inhibitors).
INVENTOR(S): Huang, Yazhong; Hu, Shuanghua; Degnan, Andrew P.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: U.S. Pat. Appl. Publ., 26 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

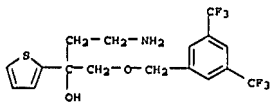
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006020019	A1	20060126	US 2005-188581	20050725
US 7179926	B2	20070220		
WO 2006014942	A1	20060209	WO 2005-US26466	20050726

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-591037P P 20040726
US 2005-188581 A 20050725

OTHER SOURCE(S): MARPAT 144:170779
IT 874469-84-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of benzyloxyalkylamines as neurokinin selective serotonin reuptake inhibitors)
RN 874469-84-8 HCAPLUS

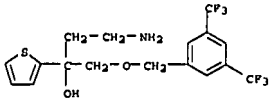
L8 ANSWER 13 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Thiophenemethanol, α-(2-aminoethyl)-α-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]- (9CI) (CA INDEX NAME)



IT 874470-88-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzyloxyalkylamines as neurokinin selective serotonin reuptake inhibitors)
RN 874470-88-9 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-α-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-, trifluoroacetate (salt) (9CI)
(CA INDEX NAME)

CM 1

CRN 874469-84-8
CMF C17 H17 F6 N O2 S

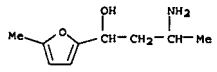


CM 2

CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

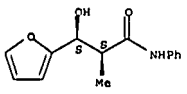
L8 ANSWER 14 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 Dec 2005
AB Synthesis of 2-(4-aza-1-hydroxy-9-iodo-3-methyl-4,9-decadienyl)-5-methylfuran for radical reaction was studied. 3-Methyl-5-(5-methyl-2-furanyl)-4,5-dihydroisoxazole was obtained from 2-methyl-5-vinylfuran. 2-(4-Iodo-4-pentenyl)-4-methyl-6-(5-methyl-2-furanyl)[1,3]oxazinane was generated by cyclization of 2-(3-amino-1-hydroxybutyl)-5-methylfuran with 5-iodo-5-hexenal. Selective protection on the amino alc. was achieved. Steric hindrance of the amino group was obstructive to a condensation reaction.
ACCESSION NUMBER: 2005:1294857 HCAPLUS
DOCUMENT NUMBER: 144:253949
TITLE: Synthesis of new furan compounds: A study towards pyrrole ring synthesis
AUTHOR(S): Karaarslan, Muhsin; Demircan, Aydin
CORPORATE SOURCE: Department of Chemistry, Faculty of Art & Science, Nigde University, Nigde, 51100, Turk.
SOURCE: Asian Journal of Chemistry (2005), Volume Date 2006, 18(1), 645-649
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:253949
IT 877437-18-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization with aldehydes)
RN 877437-18-8 HCAPLUS
CN 2-Furanmethanol, α-(2-aminopropyl)-5-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 15 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 20 Nov 2005
AB The dilithio derivs. of N-monosubstituted propanamides are formed as a mixture of stereoisomers in which the Z(O)-isomer is significantly favored by the reaction between the amide and butyllithium in THF-Et2O at 0 °C. Addition of the dilithio compound to aldehydes results in a mixture of the syn and anti aldols in near equal quantities, and in the recovery of up to 30% of the unreacted amide. The reaction outcome is essentially unaffected by time and temperature. Added zinc chloride changes the isomer ratio, but reduces chemical yields dramatically. The results are interpreted in terms of addition through three isomeric Zimmerman-Traxler-type transition states.
ACCESSION NUMBER: 2005:1226651 HCAPLUS
DOCUMENT NUMBER: 144:69425
TITLE: Addition of dilithio derivatives of N-monosubstituted propanamides to aldehydes: Stereochemistry, scope and limitations
AUTHOR(S): Gullickson, Glen C.; Khan, Mushtaq A.; Walters, Jessica A.; Baughman, Russell G.; Lewis, David E.
CORPORATE SOURCE: Department of Chemistry, University of Wisconsin - Eau Claire, Eau Claire, WI, 54702, USA
SOURCE: Synthesis (2005), (17), 2906-2912
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:69425
IT 871978-53-9P 871978-54-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereochem., scope, and limitations of addition of dilithio derivs. of N-monosubstituted propanamides to aldehydes)
RN 871978-53-9 HCAPLUS
CN 2-Furanpropanamide, β-hydroxy-α-methyl-N-phenyl-, (αR,βR)-rel- (9CI) (CA INDEX NAME)

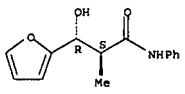
Relative stereochemistry.



RN 871978-54-0 HCAPLUS
CN 2-Furanpropanamide, β-hydroxy-α-methyl-N-phenyl-, (αR,βS)-rel- (9CI) (CA INDEX NAME)

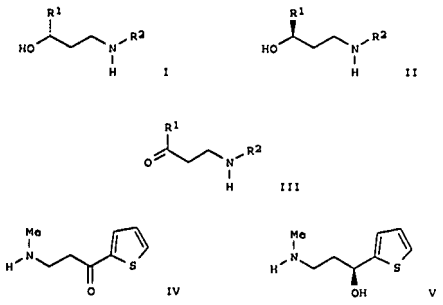
Relative stereochemistry.

L8 ANSWER 15 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 16 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 02 Sep 2005
GI



AB A process for the preparation of enantiomerically pure 1-substituted-3-aminoalcs. of formula I [wherein R1 = (un)substituted 2-thienyl, (un)substituted 2-furanyl, or (un)substituted phenyl; R2 = (un)substituted C1-4 alkyl or (un)substituted phenyl] and formula II [wherein R1 = (un)substituted 2-thienyl, (un)substituted 2-furanyl, or (un)substituted phenyl; R2 = (un)substituted C1-4 alkyl or (un)substituted phenyl], by asym. hydrogenating an aminoketone or salts of a carboxylic acid and an aminoketone of formula III [wherein R1 = (un)substituted 2-thienyl, (un)substituted 2-furanyl, or (un)substituted phenyl; R2 = (un)substituted C1-4 alkyl or (un)substituted phenyl], and wherein the corresponding aminoalcs. are obtained by subsequent hydrolysis of their salts. Thus, a mixture of 2-acetylthiophene, methylamine hydrochloride, and paraformaldehyde were heated to 120-130 °C for nine hours in ethanol and precipitated to provide 3-N-methylamino-1-(2-thienyl)-1-propanone hydrochloride (PRON-HCl, IV·HCl) which was subsequently stereoselectively reduced in the presence of a transition metal complex of a diphosphine ligand to provide (S)-(-)-3-N-methylamino-1-(2-thienyl)-1-propanol ((S)-PROL-HCl, V). Furthermore provided are salts of carboxylic acids with said aminoketones and the aminoalcs. obtained by asym. hydrogenating said aminoketones, resp.
ACCESSION NUMBER: 2005:962239 HCAPLUS
DOCUMENT NUMBER: 143:266590
TITLE: Process for the preparation of enantiomerically pure 1-substituted-3-aminoalcohols
INVENTOR(S): Michel, Dominique; Mettler, Hanspeter; McGarrity, John

L8 ANSWER 16 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080370	A1	20050901	WO 2005-EP1781	20050221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1566383	A1	20050824	EP 2004-3809	20040219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2005215906	A1	20050901	AU 2005-215906	20050221
CA 2556891	A1	20050901	CA 2005-2556891	20050221
EP 1720852	A1	20061115	EP 2005-715425	20050221
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1922168	A	20070228	CN 2005-80005452	20050221
NO 2006004017	A	20060915	NO 2006-4017	20060906

PRIORITY APPLN. INFO.: EP 2004-3809 A 20040219
EP 2004-10043 A 20040428
WO 2005-EP1781 W 20050221

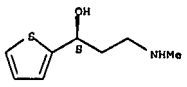
OTHER SOURCE(S): MARPAT 143:266590
IT 569687-76-9P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of enantiomerically pure 1-substituted-3-aminoalcs.)
RN 569687-76-9 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).

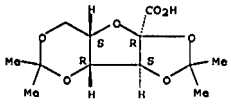
L8 ANSWER 16 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

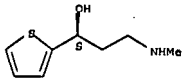
CRN 18467-77-1
CMF C12 H18 O7

Absolute stereochemistry. Rotation (-).



IT 116539-55-0P 116539-57-2P 863094-19-3P
863094-27-3P 863094-35-3P 863094-39-7P
863094-46-6P 863496-27-9P 863555-63-9P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of enantiomerically pure 1-substituted-3-aminoalcs.)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

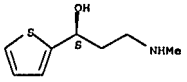
Absolute stereochemistry. Rotation (-).



RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

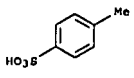
Absolute stereochemistry. Rotation (+).

L8 ANSWER 16 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 104-15-4
CMF C7 H8 O3 S

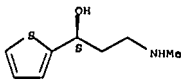


RN 863094-35-3 HCAPLUS
CN Dodecanoic acid, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).



CM 2

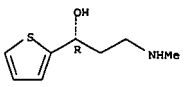
CRN 143-07-7
CMF C12 H24 O2

$HO_2C-(CH_2)_{10}-Me$

RN 863094-39-7 HCAPLUS
CN 2-Thiophenemethanol, 3-chloro-α-[2-(methylamino)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 16 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

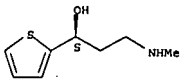


RN 863094-19-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-, benzoate (salt) (9CI) (CA INDEX NAME)

CM 1

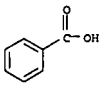
CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).



CM 2

CRN 65-85-0
CMF C7 H6 O2



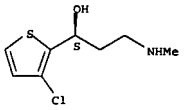
RN 863094-27-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-, 4-methylbenzenesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

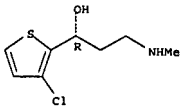
Absolute stereochemistry. Rotation (-).

L8 ANSWER 16 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

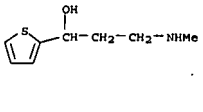


RN 863094-46-6 HCAPLUS
CN 2-Thiophenemethanol, 3-chloro-α-[2-(methylamino)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



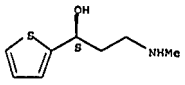
RN 863496-27-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



RN 863555-63-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, hydrochloride, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 16 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L8 ANSWER 17 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 26 Aug 2005

AB Provided is a process for the preparation of enantiomerically pure 1-substituted-3-amino alcs. (R)- or (S)-HOCH(R1)CH2CH2NHR2 (R1 = 2-thienyl, 2-furanyl, Ph, substituted 2-thienyl, substituted 2-furanyl, substituted Ph; R2 = C1-C4-alkyl, Ph, substituted C1-C4-alkyl, substituted Ph), particularly (S)-(-)- and (R)-(+)-3-N-methylamino-1-(2-thienyl)-1-propanol, by asym. hydrogenating salts of R1COCH2CH2NHR2 using Rh and an asym. ligand.

ACCESSION NUMBER: 2005:901934 HCAPLUS
DOCUMENT NUMBER: 143:248273
TITLE: Preparation of enantiomerically pure 1-substituted-3-amino alcohols
INVENTOR(S): Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: Eur. Pat. Appl., 14 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1566383	A1	20050824	EP 2004-3809	20040219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2005215906	A1	20050901	AU 2005-215906	20050221
CA 2556891	A1	20050901	CA 2005-2556891	20050221
WO 2005080370	A1	20050901	WO 2005-EP1781	20050221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1720852	A1	20061115	EP 2005-715425	20050221
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1922168	A	20070228	CN 2005-80005452	20050221
NO 2006004017	A	20060915	NO 2006-4017	20060906

PRIORITY APPLN. INFO.: EP 2004-3809 A 20040219
EP 2004-10043 A 20040428
WO 2005-EP1781 W 20050221

OTHER SOURCE(S): CASREACT 143:248273; MARPAT 143:248273

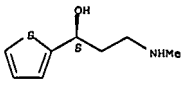
IT 116539-55-0P, (S)-(-)-3-(N-Methylamino)-1-(2-thienyl)-1-propanol
116539-57-2P 863094-39-7P 863094-46-6P

L8 ANSWER 17 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of 1-substituted -3-amino alcs. via hydrogenation of amino ketones)

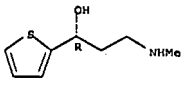
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



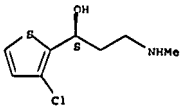
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 863094-39-7 HCAPLUS
CN 2-Thiophenemethanol, 3-chloro-α-[2-(methylamino)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

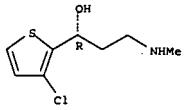
Absolute stereochemistry. Rotation (-).



RN 863094-46-6 HCAPLUS
CN 2-Thiophenemethanol, 3-chloro-α-[2-(methylamino)ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L8 ANSWER 17 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



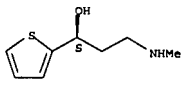
IT 569687-76-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of 1-substituted -3-amino alcs. via hydrogenation of amino ketones)

RN 569687-76-9 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

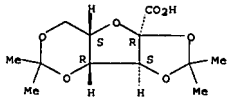
Absolute stereochemistry. Rotation (-).



CM 2

CRN 18467-77-1
CMF C12 H18 O7

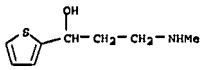
Absolute stereochemistry. Rotation (-).



IT 116539-56-1P 863094-19-3P 863094-27-3P
863094-35-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of 1-substituted -3-amino alcs. via hydrogenation of amino ketones)

RN 116539-56-1 HCAPLUS

L8 ANSWER 17 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)

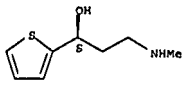


RN 863094-19-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-, benzoate (salt) (9CI) (CA INDEX NAME)

CM 1

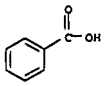
CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).



CM 2

CRN 65-85-0
CMF C7 H6 O2



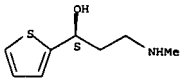
RN 863094-27-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-, 4-methylbenzenesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

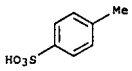
Absolute stereochemistry. Rotation (-).

L8 ANSWER 17 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 104-15-4
CMF C7 H8 O3 S

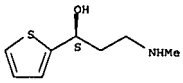


RN 863094-35-3 HCAPLUS
CN Dodecanoic acid, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).



CM 2

CRN 143-07-7
CMF C12 H24 O2

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 17 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

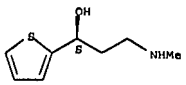
L8 ANSWER 18 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 Aug 2005
AB A process is provided for the chemoenzymic synthesis of (1S)-3-methylamino-1-(2-thienyl)-propan-1-ol from 3-chloro-1-(2-thienyl)-1-propanone using a three step procedure. First, 3-chloro-1-(2-thienyl)-1-propanone is chemical reduced to 3-chloro-1-(2-thienyl)-1-propanol using sodium borohydride. This product is then stereoselectively acylated succinic anhydride in a kinetic resolution catalyzed by an immobilized lipase. The unreacted 3S-chloro-1-(2-thienyl)-1-propanol is separated from the R conjugate base and then aminated with methylamine to form (1S)-3-methylamino-1-(2-thienyl)-propan-1-ol.
ACCESSION NUMBER: 2005:732639 HCAPLUS
DOCUMENT NUMBER: 143:192413
TITLE: A chemoenzymic synthesis of enantiomerically pure aminoalcohols
INVENTOR(S): Stuermer, Rainer
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005073215	A1	20050811	WO 2005-EP420	20050118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 102004004719	A1	20050818	DE 2004-102004004719	20040129
EP 1713788	A1	20061025	EP 2005-700995	20050118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1914190	A	20070214	CN 2005-80003670	20050118
PRIORITY APPLN. INFO.:			DE 2004-102004004719A	20040129
			WO 2005-EP420 W	20050118

OTHER SOURCE(S): CASREACT 143:192413
IT 116539-55-0P
RL: IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); PREP (Preparation)
(chemoenzymic synthesis of enantiomerically pure aminoalcs.)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 18 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L8 ANSWER 19 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005206330	A1	20050804	AU 2005-206330	20050121
CA 2553266	A1	20050804	CA 2005-2553266	20050121
EP 1711492	A1	20061018	EP 2005-701586	20050121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
CN 1910177	A	20070207	CN 2005-80002679	20050121
US 2007082895	A1	20070412	US 2006-596386	20060612
NO 2006003747	A	20060822	NO 2006-3747	20060822
PRIORITY APPLN. INFO.:			US 2004-538768P P	20040123
			WO 2005-EP50267 W	20050121

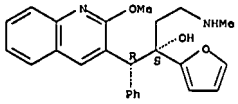
OTHER SOURCE(S): MARPAT 143:194012

IT 861709-49-1P 861709-51-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of oxazinylbenzylquinolines as mycobacterial inhibitors)

RN 861709-49-1 HCAPLUS

CN 3-Quinolineethanol, α-2-furanyl-2-methoxy-α-[2-(methylamino)ethyl]-β-phenyl-, (αR,βS)-rel- (9CI) (CA INDEX NAME)

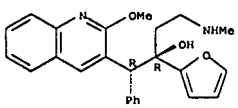
Relative stereochemistry.



RN 861709-51-5 HCAPLUS

CN 3-Quinolineethanol, α-2-furanyl-2-methoxy-α-[2-(methylamino)ethyl]-β-phenyl-, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L8 ANSWER 19 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 05 Aug 2005
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I, II; R1 = H, halo, haloalkyl, cyano, OH, Ar, Het, alkyl, alkoxy, alkylthio, alkyloxyalkyl, alkylthioalkyl, aralkyl, diarylalkyl; p = 1-4; R2 = H, OH, SH, alkoxy, alkoxyalkoxy, alkylthio, mono or dialkylamino, piperidinyl, morpholino, thiomorpholino, (alkyl)piperazinyl; R3 = alkyl, Ar, aralkyl, Het, Het-alkyl; R4 = H, alkyl, benzyl; R5 = H, halo, haloalkyl, OH, Ar, alkyl, alkoxy, alkylthio, alkoxyalkyl, alkylthioalkyl, Aralkyl, diarylalkyl; 2 vicinal R5 = atoms to form a fused Ph ring; n = 1-5; R6 = H, alkyl, Ar, Het; R7 = H, alkyl; R8 = O; or R7R8 = CH:CHN:; Z = CH2, CO; Ar = (substituted) Ph, naphthyl, acenaphthyl, tetrahydronaphthyl; Het = (substituted) N-phenoxypiperidinyl, pyrrolyl, pyrazolyl, imidazolyl, furyl, thienyl, oxazolyl, isoxazolyl, benzothiazolyl, benzothienyl, etc.], were prepared Thus, title compound (III) (prepared via cyclocondensation of paraformaldehyde with the corresponding aminoalc.) showed pIC50 = 8.5 against M. smegmatis ATCC607.

ACCESSION NUMBER: 2005:696905 HCAPLUS
DOCUMENT NUMBER: 143:194012
TITLE: Preparation of oxazinylbenzylquinolines as mycobacterial inhibitors.
INVENTOR(S): Guillemont, Jerome Emile Georges; Pasquier, Elisabeth Therese Jeanne
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070924	A1	20050804	WO 2005-EP50267	20050121
WO 2005070924	A8	20060511		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,				

L8 ANSWER 20 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 18 Jul 2005
AB The series of both syn- resp. anti-γ-thienyl-γ-hydroxy-α-aminobutanoic acids can be prepared using conjugate addition of chiral nonracemic 1-phenylethylamines on the corresponding β-thienoylacrylic acids and asym. reduction as the key steps of the synthesis. Raney nickel desulfurization in the hydrogen atmospheric represents straightforward access to the enantiomerically pure syn- resp. anti-γ-hydroxy-α-aminooctanoic resp. nonanoic acids derivs.

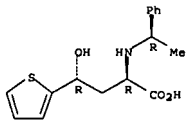
ACCESSION NUMBER: 2005:618404 HCAPLUS
DOCUMENT NUMBER: 144:253785
TITLE: Thienylsubstituted derivatives of α-aminobutanoic acid. Practical approach to enantiomerically pure γ-hydroxy-α-aminooctanoic and γ-hydroxy-α-aminononanoic acids
AUTHOR(S): Berkes, Dusan; Gubala, Vladimir; Povazanec, Frantisek
CORPORATE SOURCE: Department of Organic Chemistry, Slovak Technical University, Bratislava, SK-812 37, Slovakia
SOURCE: International Electronic Conferences on Synthetic Organic Chemistry, 5th, 6th, Sept. 1-30, 2001 and 2002 [and] 7th, 8th, Nov. 1-30, 2003 and 2004 (2004), 1393-1404. Editor(s): Seijas, Julio A. Molecular Diversity Preservation International: Basel, Switz.
CODEN: 69QTCO
DOCUMENT TYPE: Conference; (computer optical disk)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:253785

IT 877475-66-6P 877475-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzylamino(hydroxy)thienylalkanoic acids via hydrolysis of amino(thienyl)tetrahydrofuranones in the preparation of amino(hydroxy)alkanoic acid)

RN 877475-66-6 HCAPLUS

CN 2-Thiophenebutanoic acid, γ-hydroxy-α-[[(1R)-1-phenylethyl]amino]-, (αR,γR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

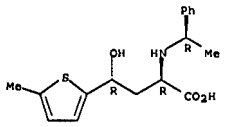


RN 877475-67-7 HCAPLUS

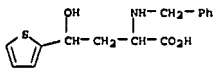
CN 2-Thiophenebutanoic acid, γ-hydroxy-5-methyl-α-[[(1R)-1-phenylethyl]amino]-, (αR,γR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L8 ANSWER 20 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

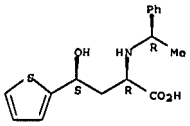


IT 877475-60-0P 877475-61-1P 877475-62-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of amino(thienyl)tetrahydrofuranones via Friedel-Crafts acylation of thiophenes with maleic anhydride followed by conjugate addition of amines, asym. reduction, and cyclization in the
preparation of amino(hydroxy) acids)
RN 877475-60-0 HCAPLUS
CN 2-Thiophenebutanoic acid, γ-hydroxy-α-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 877475-61-1 HCAPLUS
CN 2-Thiophenebutanoic acid, γ-hydroxy-α-[[(1R)-1-phenylethyl]amino]-, (αR,γS)- (9CI) (CA INDEX NAME)

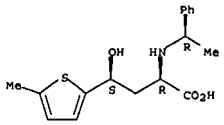
Absolute stereochemistry. Rotation (+).



RN 877475-62-2 HCAPLUS
CN 2-Thiophenebutanoic acid, γ-hydroxy-5-methyl-α-[[(1R)-1-phenylethyl]amino]-, (αR,γS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

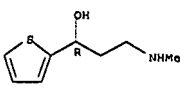
L8 ANSWER 20 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 21 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 May 2005
AB Enantioselective reduction of β-keto nitriles to optically active 1,3-amino alcs. has been carried out in one step using an excess of borane-dimethyl sulfide complex as a reductant and a polymer-supported chiral sulfonamide as a catalyst with moderate to high enantioselectivity.
The facile and enantioselective method to prepare optically active 1,3-amino
alcs. to be converted into 3-aryloxy-3-arylpropylamine-type antidepressant
drugs (R)-fluoxetine, and (R)-duloxetine is also reported.
ACCESSION NUMBER: 2005:434210 HCAPLUS
DOCUMENT NUMBER: 143:133071
TITLE: Polymer-supported chiral sulfonamide catalyzed one-pot
reduction of β-keto nitriles: a practical synthesis of (R)-fluoxetine and (R)-duloxetine
AUTHOR(S): Wang, Guangyin; Liu, Xingshun; Zhao, Gang
CORPORATE SOURCE: Laboratory of Modern Synthetic Organic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Tetrahedron: Asymmetry (2005), 16(10), 1873-1879
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:133071
IT 116539-57-2P 597581-30-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active 1,3-amino alcs. by enantioselective one-pot
reduction of β-keto nitriles catalyzed by polymer-supported chiral sulfonamide and its application in the synthesis of (R)-fluoxetine and (R)-duloxetine)
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

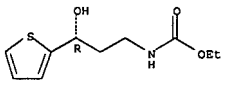
Absolute stereochemistry. Rotation (+).



RN 597581-30-1 HCAPLUS
CN Carbamic acid, [(3R)-3-hydroxy-3-(2-thienyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

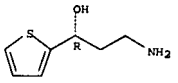
Absolute stereochemistry. Rotation (+).

L8 ANSWER 21 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



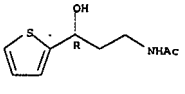
IT 858130-53-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active 1,3-amino alcs. by enantioselective one-pot
reduction of β-keto nitriles catalyzed by polymer-supported chiral sulfonamide and subsequent acylation)
RN 858130-53-7 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



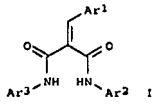
IT 858130-63-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active 1,3-amino alcs. by enantioselective one-pot
reduction of β-keto nitriles catalyzed by polymer-supported chiral sulfonamide and subsequent acylation)
RN 858130-63-9 HCAPLUS
CN Acetamide, N-[(3R)-3-hydroxy-3-(2-thienyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

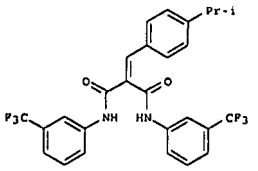


REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 22 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Apr 2005
GI



I



II

AB Substituted 2-arylmethylene-N-aryl-N'-aryl-malonamides and analogs I [wherein Ar1, Ar2, Ar3 = independently (un)substituted hetero/aryl, hetero/arylalkyl, (partially) saturated carbocyclic, heterocyclic] were prepared as activators of caspases and inducers of apoptosis for treating neoplasm.
For example, II was prepared by acylation of with 3-aminobenzotrifluoride malonyl dichloride and reaction of the diamide with 4-isopropylbenzaldehyde. II exhibited caspase activation (EC50 = 15 nM for human breast cancer cell line T-47D), inhibition of cell proliferation (GI50 = 180 nM for T-47D). II induced apoptosis in Jurkat and T-47D cells. I can be used to induce cell death in a variety of clin. conditions in which uncontrolled growth and spread of abnormal cells occurs.

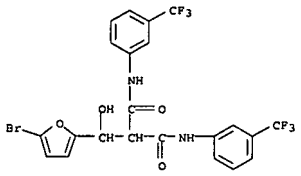
ACCESSION NUMBER: 2005:369221 HCAPLUS
DOCUMENT NUMBER: 142:430024
TITLE: Preparation of substituted 2-arylmethylene-N-aryl-N'-aryl-malonamides and analogs as activators of caspases and inducers of apoptosis
INVENTOR(S): Cai, Sui Xiong; Pervin, Azra; Kasibhatla, Shailaja; Nguyen, Bao Ngoc
PATENT ASSIGNEE(S): Cytovia, Inc., USA

L8 ANSWER 22 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
SOURCE: PCT Int. Appl., 140 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037196	A2	20050428	WO 2004-US32570	20041005
WO 2005037196	A3	20051013		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2007043076	A1	20070222	US 2006-572910	20060321

PRIORITY APPLN. INFO.: US 2003-508290P P 20031006
WO 2004-US32570 W 20041005

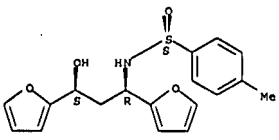
OTHER SOURCE(S): MARPAT 142:430024
IT 850798-10-6P, N,N'-Bis(3-trifluoromethylphenyl)-2-[(5-bromo-2-furyl)hydroxymethyl]malonamide
RL: SPN (Synthetic preparation); PREP (Preparation)
(drug candidate; preparation of 2-arylmethylene-N,N'-diarylmalonamides and analogs as activators of caspases and inducers of apoptosis)
RN 850798-10-6 HCAPLUS
CN Propanediamide, 2-[(5-bromo-2-furanyl)hydroxymethyl]-N,N'-bis[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 23 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 21 Apr 2005
AB The Upjohn and Donohoe dihydroxylations were exploited in divergent syntheses of aza-C-(1→1)-linked disaccharides.

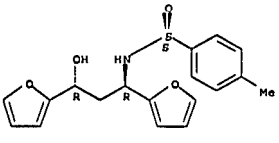
ACCESSION NUMBER: 2005:342929 HCAPLUS
DOCUMENT NUMBER: 143:26795
TITLE: A general, two-directional approach to aza-C-(1→1)-linked disaccharide mimetics
AUTHOR(S): Kennedy, Andrew; Nelson, Adam; Perry, Alexis
CORPORATE SOURCE: Synthetic Chemistry, Chemical Development, GlaxoSmithKline, Hertfordshire, SG1 2NY, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (12), 1646-1648
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:26795
IT 729567-27-5 729567-28-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(divergent preparation of aza-C-(1→1)-linked disaccharide mimetics using Upjohn and Donohoe dihydroxylations)
RN 729567-27-5 HCAPLUS
CN Benzenesulfinamide, N-[(1R,3S)-1,3-di-2-furanyl-3-hydroxypropyl]-4-methyl-, [S(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 729567-28-6 HCAPLUS
CN Benzenesulfinamide, N-[(1R,3R)-1,3-di-2-furanyl-3-hydroxypropyl]-4-methyl-, [S(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

L8 ANSWER 23 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 24 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 15 Apr 2005
AB The invention relates to enzymic and non-enzymic methods for the production of
3-methylamino-1-(thien-2-yl)propan-1-ol, o enzymes for carrying out said method, nucleic acid sequences coding for said enzymes, expression cassettes containing them, vectors and recombinant hosts. A process for preparation of 3-methylamino-1-(thien-2-yl)propan-1-ol comprises reaction of
thiophene with a β-halopropionyl halide or an acryloyl halide in the presence of a Lewis acid to obtain a 3-halo-1-(thien-2-yl)propan-1-one, reduction, and treatment with MeNH2. A hydrogen halide is added during or
after the first reaction step but before isolation of propanone product. (S)-3-methylamino-1-(thien-2-yl)propan-1-ol is prepared via treatment of the
propanone with a chiral reducing agent. Thus, thiophene in dichloroethane
was treated with AlCl3 and then with 3-chloropropionyl chloride followed by stirring for 12 h and addition of gaseous HCl to give 96% 3-chloro-1-(thien-2-yl)propan-1-one. The latter in PhMe/MeOH at 0° was treated with 30% aqueous NaOH and then with NaBH4; after 40 min. aqueous MeNH2
was added followed by stirring for 6 h at 60° to give 3-methylamino-1-(thien-2-yl)propan-1-ol.
ACCESSION NUMBER: 2005:324149 HCAPLUS
DOCUMENT NUMBER: 142:392275
TITLE: enzymic and nonenzymic methods for the preparation of 3-methylamino-1-(thien-2-yl)propan-1-ol.
INVENTOR(S): Stuermer, Rainer; Kesseler, Maria; Hauer, Bernhard; Friedrich, Thomas; Breuer, Michael
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

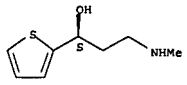
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005033094	A2	20050414	WO 2004-EP10939	20040930
WO 2005033094	A3	20051124		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10345772	A1	20050421	DE 2003-10345772	20031001
EP 1670779	A2	20060621	EP 2004-765718	20040930

L8 ANSWER 24 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

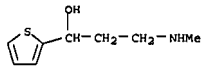
CN 1860110	A	20061108	CN 2004-80028108	20040930
US 2007083055	A1	20070412	US 2006-573130	20060517
PRIORITY APPLN. INFO.:			DE 2003-10345772 A	20031001
			WO 2004-EP10939 W	20040930

OTHER SOURCE(S): CASREACT 142:392275
IT 116539-55-0P, (S)-3-Methylamino-1-(thien-2-yl)propan-1-ol
RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

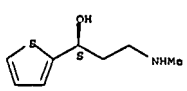


IT 116539-56-1P, 3-Methylamino-1-(thien-2-yl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(enzymic and nonenzymic methods for the preparation of methylaminothienylpropanol)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



L8 ANSWER 25 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 24 Mar 2005
AB Several β-secondary amino ketone hydrochlorides were hydrogenated with remarkably high enantioselectivities by using a rhodium complex containing P-chiral bisphospholane. These results establish a short and practical means for the synthesis of enantiopure N-monosubstituted γ-amino alcs., which are key intermediates in the synthesis of important antidepressants. For example, the bis[di(methyl)ethyl]tetra(hydro)-1,1'-bi-1H-isophosphindole-rhodium-catalyzed stereoselective hydrogenation of 3-(methylamino)-1-phenyl-1-propanone hydrochloride gave (αS)-α-[2-[(methyl)amino]ethyl]benzenemethanol, which is a synthetic precursor for (γS)-N-methyl-γ-[4-(trifluoromethyl)phenoxy]benzenepropanamine [i.e., (S)-fluoxetine]. The synthesis of (αS)-[-[(methyl)amino]ethyl]thiophenemethanol, a key synthetic intermediate for (S)-duloxetine, was also reported.
ACCESSION NUMBER: 2005:251916 HCAPLUS
DOCUMENT NUMBER: 142:481782
TITLE: Practical synthesis of enantiopure γ-amino alcohols by rhodium-catalyzed asymmetric hydrogenation of β-secondary-amino ketones
AUTHOR(S): Liu, Duan; Gao, Wenzhong; Wang, Chunjiang; Zhang, Xumu
CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Angewandte Chemie, International Edition (2005), 44(11), 1687-1689
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:481782
IT 116539-55-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (αS)-[(methyl)amino]ethyl]thiophenemethanol by bis[di(methyl)ethyl]tetra(hydro)-1,1'-bi-1H-isophosphindole-rhodium-catalyzed stereoselective hydrogenation of [(methyl)amino](thienyl)-1-propanone hydrochloride)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

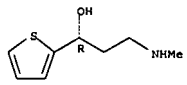
Absolute stereochemistry. Rotation (-).



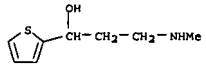
IT 116539-57-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of chiral [(methyl)amino]ethyl]arenemethanol by bis[di(methyl)ethyl]tetra(hydro)-1,1'-bi-1H-isophosphindole-rhodium-catalyzed stereoselective hydrogenation using (aryl)[(methyl)amino]propanone hydrochloride as synthetic

L8 ANSWER 25 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

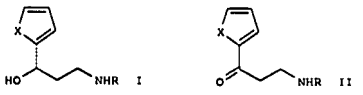
Absolute stereochemistry. Rotation (+).



IT 116539-56-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of γ-amino alc. derivative by hydrogenation of [(methyl)amino](aryl)-1-propanone hydrochloride derivative)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



L8 ANSWER 26 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 04 Mar 2005
GI



AB A process for the preparation of enantiomerically enriched or enantiomerically
pure β-amino alcs. [I; X = S, O; R = (substituted) alkyl, cycloalkyl, aryl, aralkyl] comprises asym. hydrogenation of ketones (II; variables as above) using transition metal complexes of chiral bidentate phosphines as catalysts. Thus, 3-methylamino-1-(thien-2-yl)propan-1-one hydrochloride (preparation given), NaOMe, (S,S)-Me-DuPhos, and [Rh(COD)2]BF4 were autoclaved
together in MeOH at 30-34° and 30 bar H2 for 5 h to give 67% (S)-3-methylamino-1-(2-thienyl)-1-propanol in >99% enantiomeric excess.
ACCESSION NUMBER: 2005:181066 HCAPLUS
DOCUMENT NUMBER: 142:280046
TITLE: Process for the asymmetric hydrogenation of β-amino ketones using transition metal complexes of chiral bidentate phosphines as catalysts.
PATENT ASSIGNEE(S): Lonza AG, Switz.
SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1510517	A1	20050302	EP 2003-77734	20030901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004268057	A1	20050310	AU 2004-268057	20040831
WO 2005021527	A2	20050310	WO 2004-EP9690	20040831
WO 2005021527	A3	20050714		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

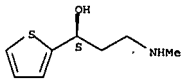
L8 ANSWER 26 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

EP 1664014	A2	20060607	EP 2004-764655	20040831
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1842523	A	20061004	CN 2004-80024598	20040831
JP 2007504192	T	20070301	JP 2006-525092	20040831
NO 2006000763	A	20060317	NO 2006-763	20060217
US 2006252945	A1	20061109	US 2006-569824	20060228

PRIORITY APPLN. INFO.: EP 2003-77734 A 20030901
WO 2004-EP9690 W 20040831

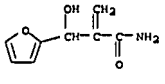
OTHER SOURCE(S): CASREACT 142:280046; MARPAT 142:280046
IT 116539-55-0P, (S)-3-Methylamino-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(asym. hydrogenation of aminoketones using transition metal complexes of chiral bidentate phosphines as catalysts)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 27 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 17 Jan 2005
AB Novel aprotic polar solvents are selected for use towards a facile Baylis-Hillman reaction, catalyzed by the standard base (DABCO), so that less
reactive aldehydes and a broad spectrum of activated olefins (including acrylamide) could be coupled under the altered reaction conditions.
ACCESSION NUMBER: 2005:38955 HCAPLUS
DOCUMENT NUMBER: 142:176427
TITLE: Novel aprotic polar solvents for facile Baylis-Hillman reaction
AUTHOR(S): Krishna, Palakodety Radha; Manjuvani, A.; Sekhar, Empati Raja
CORPORATE SOURCE: Discovery Laboratory, Organic Chemistry Division-III, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SOURCE: ARKIVOC (Gainesville, FL, United States) (2005), (3), 99-109
CODEN: AGFUAR
URL: http://www.arkat-usa.org/ark/journal/2005/I03_Rao/1203/1203.pdf
PUBLISHER: Arkat USA Inc.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:176427
IT 497221-43-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of hydroxyalkenoates via Baylis-Hillman reaction of aldehydes
with acrylates in sulfolane, N-methylmorpholine, or N-methylpyrrolidinone)
RN 497221-43-9 HCAPLUS
CN 2-Furanpropanamide, β-hydroxy-α-methylene- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

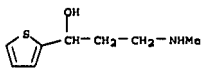
L8 ANSWER 28 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 03 Dec 2004
AB There is provided a process for producing an optically active N-monoalkyl-3-oxo-3-arylpropylamine compound represented by the formula ArC*H(OH)CH2CH2NHR1 (wherein symbol * indicates an asym. carbon atom; R1 represents optionally substituted C1-5 alkyl; Ar represents optionally substituted aryl or heteroaryl) characterized by asym. reducing a (Z)-protected-N-monoalkyl-3-oxo-3-arylpropenylamine compound represented by
the formula (Z)-ArCOCH:CHNR1R2 (wherein Ar and R1 are same as defined above; R2 represents an amino-protecting group) with an asym. catalyst to give an optically active compound represented by the formula ArC*H(OH)CH2CH2NR1R2 (wherein the symbol *, Ar, R1, and R2 are same as defined above) and successively eliminating the protective group (R2). Thus, 16.7 g (Z)-N-methyl-3-oxo-3-(2-thienyl)propenylamine was acylated by
16.4 g iso-Bu chlorocarbonate in the presence of 1.2 g 4-dimethylaminopyridine and 12.1 g Et3N in 200 mL tert-Bu Me ether at 50° for 28 h to give 22.0 g N-methyl-N-isobutoxycarbonyl-[(Z)-3-oxo-3-(2-thienyl)propenyl]amine (I). I (33.8 mg) was stirred in 2-propanol in
the presence of potassium tert-butoxide and 2.3 mg [(S)-N-phenyl-2-azetidinecarboxamide]ruthenium(p-cymene) chloride (REG 543689-61-8) at 80° for 4 h to give 84% N-methyl-N-isobutoxycarbonyl-3-hydroxy-3-(2-thienyl)propylamine which (114.8 mg) was treated with a mixture of 0.2 g 30
weight% aqueous NaOH and 5 mL 2-propanol at 30° for 24 h to give N-methyl-3-hydroxy-3-(2-thienyl)propylamine (50% ee).
ACCESSION NUMBER: 2004:1037091 HCAPLUS
DOCUMENT NUMBER: 142:23180
TITLE: Process for producing optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound and intermediate
INVENTOR(S): Iwakura, Kazunori; Higashii, Takayuki; Bando, Seiji
PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co. Ltd., Japan
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004103990	A1	20041202	WO 2004-JP6602	20040511
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004346008	A	20041209	JP 2003-144742	20030522

PRIORITY APPLN. INFO.: JP 2003-144742 A 20030522

OTHER SOURCE(S): CASREACT 142:23180; MARPAT 142:23180

L8 ANSWER 28 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 116539-56-1P, N-Methyl-[3-hydroxy-3-(2-thienyl]propyllamine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound by asym. reduction of aminovinyl aryl or heteroaryl ketone and deprotection)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

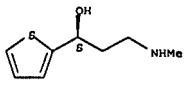
L8 ANSWER 29 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 21 Oct 2004
AB The present invention concerns proteins, which possess an enzymic activity for reduction of substituted alkanones, such as 3-methylamino-1-(2-thienyl)-propane-1-one. Furthermore, the invention concerns nucleic acids which code for these proteins, vectors, and genetically modified microorganisms as well as procedures for the production of substituted (S)-alkanols, e.g., (S)-3-methylamino-1-(2-thienyl)-(S)-propanol. This compound may be used in the synthesis of duloxetine.
ACCESSION NUMBER: 2004:870926 HCAPLUS
DOCUMENT NUMBER: 141:348875
TITLE: L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols
INVENTOR(S): Althoefer, Henning; Kesseler, Maria
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 41 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10315760	A1	20041021	DE 2003-10315760	20030407
CA 2521288	A1	20041021	CA 2004-2521288	20040406
WO 2004090094	A2	20041021	WO 2004-EP3655	20040406
WO 2004090094	A3	20050317		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1613745	A2	20060111	EP 2004-725924	20040406
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1771323	A	20060510	CN 2004-80009243	20040406
JP 2006521800	T	20060928	JP 2006-505019	20040406
US 2006211099	A1	20060921	US 2005-552218	20051006

PRIORITY APPLN. INFO.: DE 2003-10315760 A 20030407
WO 2004-EP3655 W 20040406

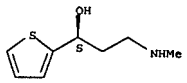
L8 ANSWER 29 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
OTHER SOURCE(S): CASREACT 141:348875
IT 116539-55-0P
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(l-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 30 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 21 Sep 2004
AB On page 3841, Introduction, line 14 should read: "The proposed major metabolites found in human plasma were the glucuronide conjugates of 4-hydroxyduloxetine, 6-hydroxy-5-methoxyduloxetine, 4,6-dihydroxyduloxetine, and the sulfate conjugate or 5-hydroxy-6-methoxyduloxetine.". On page 3486, the sentence beginning on line 23 should read: "Compound 2 had moderate to weak activity in all of the membranes; however, this compound is unstable so the values may not be accurate.". Two subsequent sentences are added: "Although compounds 2, 3, 4, and 7 showed some degree of in vitro affinity, these compounds do not appear to contribute to the in vivo activity of duloxetine, since they circulate in human plasma at such low concentrations. The circulating metabolites are in the conjugated forms and do not appear to be active.". The last sentence of the paragraph should read: "The conjugated metabolites tested (10, 11, 12, 13, 15) were devoid of any significant binding to any of the three transporters.".
ACCESSION NUMBER: 2004:767311 HCAPLUS
DOCUMENT NUMBER: 142:336194
TITLE: Synthesis and biological activity of some known and putative duloxetine metabolites. [Erratum to document cited in CA141:206997]
AUTHOR(S): Kuo, F.; Gillespie, T. A.; Kulanthaivel, P.; Lantz, R. J.; Ma, T. W.; Nelson, D. L. G.; Threlkeld, P. G.; Wheeler, W. J.; Yi, P.; Zmijewski, M.
CORPORATE SOURCE: Lilly Research Laboratories, Lilly Corporate Center, Eli Lilly and Company, Indianapolis, IN, 46285, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(20), 5233
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 116539-55-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of duloxetine metabolites and study of their ability to inhibit radioligand binding to human serotonin, norepinephrine, and dopamine transporters (Erratum))
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



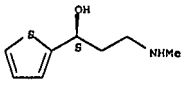
L8 ANSWER 31 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Jul 2004
AB 3-Methylamino-1-(2-thienyl)-1-propanone and its acid addition salts (e.g., the hydrochloride), which are useful as an intermediate in the production of the pharmaceutical (+)-(S)-N-methyl-3-(1-naphthyloxy)-3-(2-thienyl)propylamine oxalate (i.e., Duloxetine oxalate), are prepared
ACCESSION NUMBER: 2004:605494 HCAPLUS
DOCUMENT NUMBER: 141:140312
TITLE: 3-Methylamino-1-(2-thienyl)-1-propanone preparation and its use as a pharmaceutical intermediate
PATENT ASSIGNEE(S): BASF Ag, Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10302595	A1	20040729	DE 2003-10302595	20030122
CA 2513542	A1	20040805	CA 2004-2513542	20040115
WO 2004065376	A1	20040805	WO 2004-EP237	20040115
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ				
EP 1587802	A1	20051026	EP 2004-702333	20040115
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1742003	A	20060301	CN 2004-80002686	20040115
JP 2006515878	T	20060608	JP 2006-500570	20040115
US 2006128791	A1	20060615	US 2005-542003	20050712

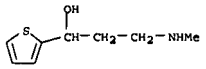
PRIORITY APPLN. INFO.: DE 2003-10302595 A 20030122
WO 2004-EP237 W 20040115

IT 116539-55-0P 116539-56-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

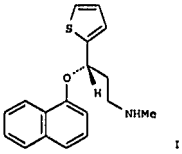
Absolute stereochemistry. Rotation (-).



L8 ANSWER 31 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



L8 ANSWER 32 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 10 Jun 2004
GI

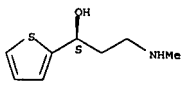


I

AB Several putative phase I duloxetine (I) metabolites, 4-hydroxy-, 5-hydroxy-, 6-hydroxy-, 5-hydroxy-6-methoxy-, 6-hydroxy-5-methoxy-, 5,6-dihydroxy-, and 4,6-dihydroxyduloxetine were synthesized, and their phase II metabolite as glucuronide or sulfate conjugates were also synthesized. Their in vitro binding activities were compared to that of parent compound duloxetine; they were evaluated for their ability to inhibit radioligand binding to human serotonin, norepinephrine, and dopamine transporters.
ACCESSION NUMBER: 2004:465496 HCAPLUS
DOCUMENT NUMBER: 141:206997
TITLE: Synthesis and biological activity of some known and putative duloxetine metabolites
AUTHOR(S): Kuo, P.; Gillespie, T. A.; Kulanthaivel, P.; Lantz, R. J.; Ma, T. W.; Nelson, D. L.; Threlkeld, P. G.; Wheeler, W. J.; Yi, P.; Zmijewski, M.
CORPORATE SOURCE: Lilly Corporate Center, A Division of Eli Lilly and Company, Lilly Research Laboratories, Indianapolis, IN, 46285, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(13), 3481-3486
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:206997
IT 116539-55-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of duloxetine metabolites and study of their ability to inhibit radioligand binding to human serotonin, norepinephrine, and dopamine transporters)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

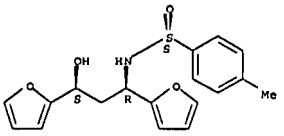
L8 ANSWER 32 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 33 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 28 May 2004
AB Lithium enolates derived from ketones may be added to N-sulfinylimines with high diastereoselectivity. Diastereoselective reduction gave either the syn- or anti-1,3-amino alc. derivative
ACCESSION NUMBER: 2004:434662 HCAPLUS
DOCUMENT NUMBER: 141:156976
TITLE: Highly diastereoselective addition of ketone enolates to N-sulfinyl imines: Asymmetric synthesis of syn- and anti-1,3-amino alcohol derivatives
AUTHOR(S): Kennedy, Andrew; Nelson, Adam; Perry, Alexis
CORPORATE SOURCE: GlaxoSmithKline, Kent, TN11 9AN, UK
SOURCE: Synlett (2004), (6), 967-970
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:156976
IT 729567-27-5P 729567-28-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective addition of ketone enolates to N-sulfinylimines in asym. synthesis of syn- and anti-1,3-amino alcs.)
RN 729567-27-5 HCAPLUS
CN Benzenesulfinamide, N-[(1R,3S)-1,3-di-2-furanyl-3-hydroxypropyl]-4-methyl-, [S(S)]- (9CI) (CA INDEX NAME)

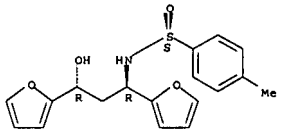
Absolute stereochemistry. Rotation (+).



RN 729567-28-6 HCAPLUS
CN Benzenesulfinamide, N-[(1R,3R)-1,3-di-2-furanyl-3-hydroxypropyl]-4-methyl-, [S(S)]- (9CI) (CA INDEX NAME)

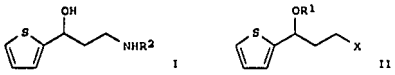
Absolute stereochemistry. Rotation (+).

L8 ANSWER 33 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 34 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 06 May 2004
GI

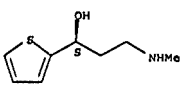


AB Title compds. (I; R2 = alkyl, aralkyl, aryl) were prepared by reacting II (X = Cl, Br; R1 = H, acyl, silyl) with an amine R2NH2 (R2 as above) in a closed system at 0°-400°. Thus, 3-chloro-1-(2-thienyl)-1-propanol in THF was added to an aqueous solution of MeNH2 followed by heating at 80° for 5 h to give 68% 3-methylamino-1-(2-thienyl)-1-propanol with a purity of >99%.
ACCESSION NUMBER: 2004:367200 HCAPLUS
DOCUMENT NUMBER: 140:357199
TITLE: Procedure for the production of thienyl-substituted secondary aminoalcohols
INVENTOR(S): Heldmann, Dieter; Stohrer, Juergen
PATENT ASSIGNEE(S): Consortium Fuer Elektrochemische Industrie GmbH, Germany
SOURCE: Ger. Offen., 5 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

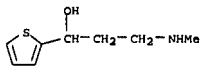
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10248480	A1	20040506	DE 2002-10248480	20021017
PRIORITY APPLN. INFO.:			DE 2002-10248480	20021017

OTHER SOURCE(S): MARPAT 140:357199
IT 116539-55-0P 116539-56-1P, 3-Methylamino-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(procedure for production of thienyl-substituted secondary aminoalcs.)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

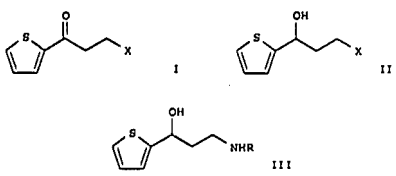
Absolute stereochemistry. Rotation (-).



L8 ANSWER 34 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



L8 ANSWER 35 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 06 May 2004
GI

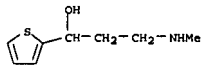


AB Thienyl-substituted β-haloketones (I; X = Br, Cl) were prepared by reacting thiophene with an acid halide XCH2CH2C(O)Cl (X as above) in the presence of a Friedel-Crafts catalyst selected from organic or inorg. acids, metals, perchlorates, H3PO4 derivs., or halides. The reaction is carried out in such a way that the Friedel-Crafts catalyst is treated with the thiophene and an acid halide. The invention relates as well as preparation of thienyl-substituted secondary aminoalcs. (III; R = alkyl, aralkyl, aryl) by (1) reduction of I to II (X as above), and (2) reacting II with RNH2 (R as above) in a closed system at 0°-400°. Thus, a suspension of AlCl3 in CH2Cl2 was cooled in an ice bath followed by dropwise treatment with 3-chloropropionyl chloride and subsequently with thiophene at <20°. The reaction mixture was stirred for 1 h at room temperature to give 87% 3-chloro-1-(2-thienyl)-1-propanone. 3-Chloro-1-(2-thienyl)-1-propanol (preparation given) and MeNH2 in THF were heated at 80° for 5 h to give 68% 3-methylamino-1-(2-thienyl)-1-propanol with a purity of >99%.

ACCESSION NUMBER: 2004:367199 HCAPLUS
DOCUMENT NUMBER: 140:357198
TITLE: Procedure for the production of thienyl-substituted secondary aminoalcohols
INVENTOR(S): Heldmann, Dieter; Stohrer, Juergen; Zauner, Raffael
PATENT ASSIGNEE(S): Consortium Fuer Elektrochemische Industrie GmbH, Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

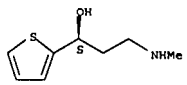
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10248479	A1	20040506	DE 2002-10248479	20021017
PRIORITY APPLN. INFO.:			DE 2002-10248479	20021017

OTHER SOURCE(S): CASREACT 140:357198; MARPAT 140:357198
IT 116539-56-1P, 3-Methylamino-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(procedure for production of thienyl-substituted secondary aminoalcs.)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)

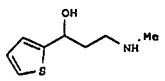


IT 116539-55-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(procedure for production of thienyl-substituted secondary aminoalcs.)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 36 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Apr 2004
GI



AB Optically active 3-(methylamino)-1-(2-thienyl)propan-1-ol (I), useful as an intermediate for duloxetine, is prepared by optical resolution of its racemate using optically active mandelic acids or tartaric acids. (RS)-I was treated with (S)-mandelic acid in 2-butanol under heating and cooled to give 66.4% (S)-I.(S)-mandelate.H2O, which was treated with NaOH in H2O/2-butanol to give 66% (S)-I with 99.9% ee.

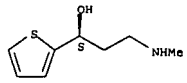
ACCESSION NUMBER: 2004:330162 HCAPLUS
DOCUMENT NUMBER: 140:339189
TITLE: Preparation of optically active (methylamino)thienylpropanol and its intermediate diastereomer salts
INVENTOR(S): Sakai, Kenichi; Sakurai, Rumiko; Yuzawa, Mutsumi; Hatahira, Kaoru
PATENT ASSIGNEE(S): Yamakawa Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004123596	A	20040422	JP 2002-289068	20021001
US 2006063943	A1	20060323	US 2004-947333	20040923
US 7119211	B2	20061010		
PRIORITY APPLN. INFO.:			JP 2002-289068 A	20021001

OTHER SOURCE(S): MARPAT 140:339189
IT 116539-55-0P, (S)-3-(Methylamino)-1-(2-thienyl)propan-1-ol
RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(optical resolution of (methylamino)thienylpropanol using mandelic acids or tartaric acids)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 36 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

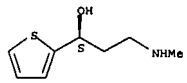


IT 586968-36-7P 680624-70-8P 680624-71-9P
680624-72-0P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(optical resolution of (methylamino)thienylpropanol using mandelic acids or tartaric acids)
RN 586968-36-7 HCAPLUS
CN Benzeneacetic acid, α-hydroxy-, (αS)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

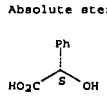
Absolute stereochemistry. Rotation (-).



CM 2

CRN 17199-29-0
CMF C8 H8 O3

Absolute stereochemistry. Rotation (+).



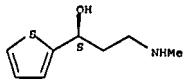
RN 680624-70-8 HCAPLUS
CN Benzeneacetic acid, α-methoxy-, (αR)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

L8 ANSWER 36 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

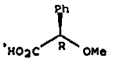
Absolute stereochemistry. Rotation (-).



CM 2

CRN 3966-32-3
CMF C9 H10 O3

Absolute stereochemistry. Rotation (-).

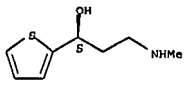


RN 680624-71-9 HCAPLUS
CN Butanedioic acid, 2,3-bis[(4-methylbenzoyl)oxy]-, (2R,3R)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).

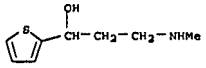


CM 2

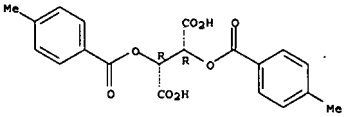
CRN 32634-66-5
CMF C20 H18 O8

Absolute stereochemistry. Rotation (-).

L8 ANSWER 36 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(optical resoln. of (methylamino)thienylpropanol using mandelic acids or tartaric acids)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



L8 ANSWER 36 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

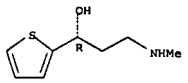


RN 680624-72-0 HCAPLUS
CN Butanedioic acid, 2,3-bis(benzoyloxy)-, (2R,3R)-, compd. with (αR)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-57-2
CMF C8 H13 N O S

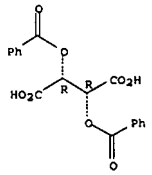
Absolute stereochemistry. Rotation (+).



CM 2

CRN 2743-38-6
CMF C18 H14 O8

Absolute stereochemistry. Rotation (-).



IT 116539-56-1, 3-(Methylamino)-1-(2-thienyl)propan-1-ol
RL: RCT (Reactant); RACT (Reactant or reagent)

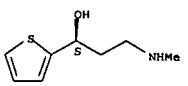
L8 ANSWER 37 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2004
AB Optically active R1CH(OH)CHR2CHR3NHR4 [R1 = (substituted) hydrocarbyl, heteroaryl, heterocyclyl; R2, R3 = H, (substituted) hydrocarbyl, acyl, acyloxy, alkoxycarbonyl, aralkoxycarbonyl, aryloxycarbonyl, heteroaryl, heterocyclyl; R4 = H, protecting group; ≥2 of R1-R4 may be bonded to each other to form a ring; with provisos], were prepared by asym. hydrogenation of cis- or trans-R1COCR2:CR3NHR4 (variables as above). Thus, 3-methylamino-1-thiophen-2-ylpropenone, RuCl2[(R)-DM-binap][(R)-daipen] [DM-binap = 2,2'-bis(bis(3,5-dimethylphenyl)phosphino)-1,1'-binaphthyl; daipen = 1,2-di(4-anisyl)-2-isopropyl-1,2-ethylenediamine], and K2CO3 in Me2CHOH were autoclaved under 2.5 MPa H2 at 30° for 18 h to give 79.2% (S)-3-methylamino-1-(2-thienyl)propan-1-ol.

ACCESSION NUMBER: 2004:326179 HCAPLUS
DOCUMENT NUMBER: 140:339187
TITLE: Preparation of optically active amino alcohols by asymmetric hydrogenation of enaminones.
INVENTOR(S): Yokozawa, Tohru; Yagi, Kenji; Saito, Takao
PATENT ASSIGNEE(S): Japan
SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1411045	A1	20040421	EP 2003-23628	20031016
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004155770	A	20040603	JP 2003-339801	20030930
US 2004082794	A1	20040429	US 2003-686598	20031017
US 6984738	B2	20060110		
PRIORITY APPLN. INFO.:			JP 2002-305147 A	20021018

OTHER SOURCE(S): MARPAT 140:339187
IT 116539-55-0P, (S)-3-Methylamino-1-(2-thienyl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active amino alcs. by asym. hydrogenation of enaminones)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

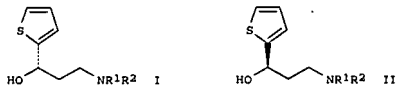
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 37 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L8 ANSWER 38 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 15 Apr 2004
GI



AB Title compds. (I, II; R1, R2 = H, alkyl, cycloalkyl, aralkyl, aryl), were prepared by reducing the corresponding 3-amino-1-(2-thienyl)-1-propanones using a hydrogen donor in the presence of a metal catalyst, an optically active N-containing ligand and optionally a base. Thus, 3-N-methylamino-1-(2-thienyl)-1-propanone hydrochloride (preparation given) and NaOH were stirred 1 h in Me2CHOH; a prestirred solution of (1S,2R)-cis-1-amino-2-indanol and (p-cymene)ruthenium(II)chloride dimer in Me2CHOH was added followed by stirring for 4 h at 20° to give 39% (S)-N-methylamino-1-(2-thienyl)-1-propanol in 70% enantiomeric excess.

ACCESSION NUMBER: 2004:308427 HCAPLUS
DOCUMENT NUMBER: 140:321232
TITLE: Preparation of optically active 3-amino-1-(2-thienyl)-1-propanols via reduction of 3-amino-1-(2-thienyl)-1-propanones using a hydrogen donor in the presence of a metal catalyst, an optically active nitrogen-containing ligand and optionally a base.
INVENTOR(S): Fuchs, Rudolf; Michel, Dominique; Brieden, Walter
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031168	A2	20040415	WO 2003-EP11073	20031007
WO 2004031168	A3	20040826		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ; OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,

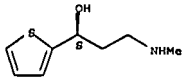
L8 ANSWER 38 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003276066	A1	20040423	AU 2003-276066	20031007
PRIORITY APPLN. INFO.:			EP 2002-22540	A 20021007
			WO 2003-EP11073	W 20031007

OTHER SOURCE(S): CASREACT 140:321232; MARPAT 140:321232

IT 116539-55-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active aminothienylpropanols via reduction of aminothienylpropanones using a hydrogen donor in the presence of a metal catalyst, an optically active N-containing ligand and a base)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

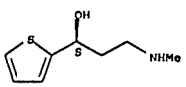


IT 569687-76-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active aminothienylpropanols via reduction of aminothienylpropanones using a hydrogen donor in the presence of a metal catalyst, an optically active N-containing ligand and a base)
RN 569687-76-9 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

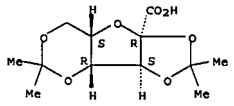
Absolute stereochemistry. Rotation (-).



CM 2

L8 ANSWER 38 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 18467-77-1
CMF C12 H18 O7

Absolute stereochemistry. Rotation (-).



L8 ANSWER 39 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 08 Apr 2004
AB A process for the production of 3-heteroaryl-3-hydroxy-propionic acid derivs.
by enantioselective microbial reduction is provided. Thus, Saccharomyces cerevisiae was used to reduce methyl-3-oxo-3-(2-thiophenyl)propanoic acid to methyl-(3S)-hydroxy-3-(2-thiophenyl)propanoic acid with a yield of 75% and an enantiomeric excess >97%. The reaction product then served as a reactant in the chemical synthesis of (1S)-3-(methylamino)-1-(2-thienyl)-1-propanol.
ACCESSION NUMBER: 2004:286808 HCAPLUS
DOCUMENT NUMBER: 140:302436
TITLE: Process for the production of 3-heteroaryl-3-hydroxy-propionic acid derivatives by enantioselective microbial reduction
INVENTOR(S): Berendes, Frank; Eckert, Markus; Brinkmann, Nils; Dreisbach, Claus; Meissner, Ruth; Koch, Rainhard
PATENT ASSIGNEE(S): Bayer Chemicals A.-G., Germany
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

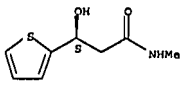
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1405917	A2	20040407	EP 2003-20847	20030913
EP 1405917	A3	20050112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10244811	A1	20040408	DE 2002-10244811	20020926
IN 2003MU00922	A	20050715	IN 2003-MU922	20030908
US 2004181058	A1	20040916	US 2003-669424	20030924
JP 2004113245	A	20040415	JP 2003-335690	20030926
CN 1497048	A	20040519	CN 2003-160307	20030926
US 2006264641	A1	20061123	US 2006-436347	20060518

PRIORITY APPLN. INFO.: DE 2002-10244811 A 20020926
US 2003-669424 A3 20030924

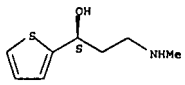
OTHER SOURCE(S): MARPAT 140:302436
IT 116539-55-0P 116539-57-2P, (1R)-3-(Methylamino)-1-(2-thienyl)-1-propanol 603959-56-4P, (S)-3-Hydroxy-3-(2-thienyl)propanoic acid N-methylamide
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(process for production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by
enantioselective microbial reduction)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 39 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

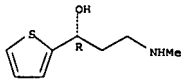


L8 ANSWER 39 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



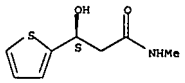
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 603959-56-4 HCAPLUS
CN 2-Thiophenepropanamide, β-hydroxy-N-methyl-, (βS)- (9CI) (CA INDEX NAME)

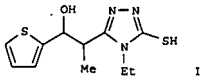
Absolute stereochemistry. Rotation (-).



IT 603959-56-4DP, N-methyl-(3S)-3-hydroxy-3-(2-thienyl)propanamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for production of 3-heteroaryl-3-hydroxy-propionic acid derivs. by
enantioselective microbial reduction)
RN 603959-56-4 HCAPLUS
CN 2-Thiophenepropanamide, β-hydroxy-N-methyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

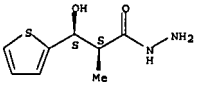
L8 ANSWER 40 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 05 Apr 2004
GI



I

AB The synthesis, spectral properties, and relative configuration of new diastereoisomeric 1-(2-thienyl)-alcs. containing 4(H)-1,2,4-triazole derivs., e.g., I, and their cytotoxicity are reported. In particular the effect of substitution and relative configuration upon the cytotoxic-activity against myeloid tumor cells induced by Graffi virus is discussed.
ACCESSION NUMBER: 2004:277385 HCAPLUS
DOCUMENT NUMBER: 142:56238
TITLE: Synthesis and cytotoxicity of new diastereoisomeric 1-(2-thienyl)-2-(1,2,4-triazol-3-yl)-alkanols
AUTHOR(S): Mavrova, A.; Wesselinova, D.
CORPORATE SOURCE: University of Chemical Technology and Metallurgy, Sofia, 1756, Bulg.
SOURCE: Dokladi na Bulgarskata Akademiya na Naukite (2003), 56(7), 59-64
CODEN: DBANEH; ISSN: 0861-1459
PUBLISHER: Bulgarska Akademiya na Naukite
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:56238
IT 474900-73-7 474900-75-9 474900-77-1 474900-79-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation antitumor activity, and SAR of thienyl(triazolyl)alkanols via addition of thienyl(hydrazinocarbonyl)alkanols to carbon disulfide followed by heterocyclization with hydrazine and methylation)
RN 474900-73-7 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, hydrazide, (αR,βR)-rel- (9CI) (CA INDEX NAME)

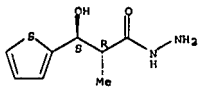
Relative stereochemistry.



RN 474900-75-9 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, hydrazide, (αR,βS)-rel- (9CI) (CA INDEX NAME)

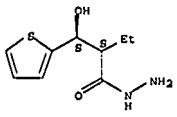
Relative stereochemistry.

L8 ANSWER 40 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



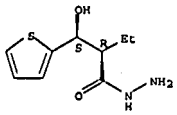
RN 474900-77-1 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, hydrazide, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 474900-79-3 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, hydrazide, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

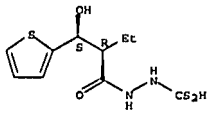


IT 809236-56-4P 809236-57-5P 809236-59-7P
809236-60-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation antitumor activity, and SAR of thienyl(triazolyl)alkanols via addition of thienyl(hydrazinocarbonyl)alkanols to carbon disulfide followed by heterocyclization with hydrazine and methylation)
RN 809236-56-4 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, 2-(dithiocarboxy)hydrazide, monopotassium salt, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 40 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
2-(dithiocarboxy)hydrazide, monopotassium salt, (αR,βS)-rel- (9CI) (CA INDEX NAME)

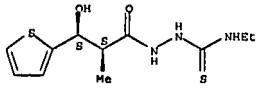
Relative stereochemistry.



● K

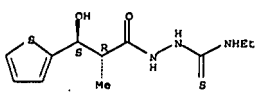
IT 809236-68-8P 809236-69-9P
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, antitumor activity, and SAR of thienyl(triazolyl)alkanols via addition of thienyl(hydrazinocarbonyl)alkanols to Et isothiocyanate followed by heterocyclization)
RN 809236-68-8 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, 2-[(ethylamino)thioxomethyl]hydrazide, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



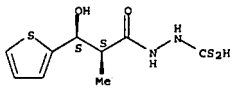
RN 809236-69-9 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, 2-[(ethylamino)thioxomethyl]hydrazide, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR

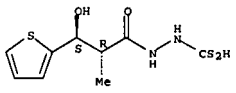
L8 ANSWER 40 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● K

RN 809236-57-5 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, 2-(dithiocarboxy)hydrazide, monopotassium salt, (αR,βS)-rel- (9CI) (CA INDEX NAME)

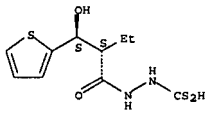
Relative stereochemistry.



● K

RN 809236-59-7 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, 2-(dithiocarboxy)hydrazide, monopotassium salt, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

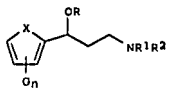


● K

RN 809236-60-0 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-,

L8 ANSWER 40 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 41 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 26 Mar 2004
GI



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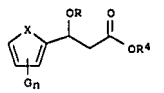


II

AB Title compds. [I; X = S, O, NR3; R3 = H, organic group; R = H, organic group;
R1, R2 = H, (substituted) alkyl, aryl; G = substituent; n = 0-3], were prepared by reaction of ester [II; R4 = (substituted) alkyl, alkenyl, alkynyl, aryl, heteroaryl; other variables as above] with NHR1R2 to give the corresponding amide, followed by reduction Thus, Et (S)-3-hydroxy-3-(2-thienyl)propanoate (preparation given) was stirred 1 h with MeNH2 in PhMe to give 36% (S)-N-Methyl-3-hydroxy-3-(2-thienyl)propanamide. The latter in THF was treated with LiAlH4 in THF to give 88% (S)-3-methylamino-1-(2-thienyl)propan-1-ol.

ACCESSION NUMBER: 2004:252497 HCAPLUS
DOCUMENT NUMBER: 140:287257
TITLE: Process for the preparation of heterocyclic hydroxypropylamines via amidation and reduction of the corresponding esters.
INVENTOR(S): Houson, Ian Nicholas
PATENT ASSIGNEE(S): Avecia Limited, UK
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

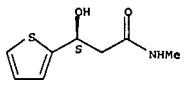
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004024708	A2	20040325	WO 2003-GB3982	20030912
WO 2004024708	A3	20040603		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2498756	A1	20040325	CA 2003-2498756	20030912

L8 ANSWER 41 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AU 2003271844	A1	20040430	AU 2003-271844	20030912
EP 1542985	A2	20050622	EP 2003-753682	20030912
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1694878	A	20051109	CN 2003-825120	20030912
JP 2006513145	T	20060420	JP 2004-535693	20030912
NO 2005001240	A	20050401	NO 2005-1240	20050310
US 2005272940	A1	20051208	US 2005-528092	20050316
PRIORITY APPLN. INFO.:			GB 2002-21438 A	20020916
			WO 2003-GB3982 W	20030912

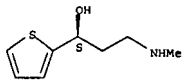
OTHER SOURCE(S): CASREACT 140:287257; MARPAT 140:287257
IT 603959-56-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic hydroxypropylamines via amidation and reduction of the corresponding esters)
RN 603959-56-4 HCAPLUS
CN 2-Thiophenepropanamide, β-hydroxy-N-methyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

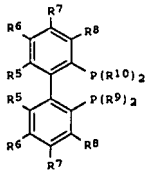


IT 116539-55-0P, (S)-3-Methylamino-1-(2-thienyl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of heterocyclic hydroxypropylamines via amidation and reduction of the corresponding esters)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 42 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 14 Mar 2004
GI



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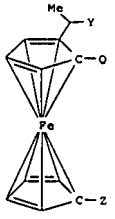


II

AB The invention relates to methods for the enantioselective production of amino alcs., R1CH(OH)CH2(CH2)nNHR2 [R1 = (un)substituted, (un)saturated or aromatic carbocycle or heterocycle (optionally substituted with R3, R4); R2 = H, C1-20-alkyl; R3, R4 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, CO2R2, F, Cl, Br, OH, CN, NO2, N(R2)2, NHCOR2; n = 0 - 3], via the enantioselective hydrogenation of amino ketones, R1COCH2(CH2)nNHR2 and is characterized by hydrogenation in the presence of a non-racemic catalyst containing a chiral diphosphine ligand I [R5, R6, R7, R8 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, F, Cl, Br, N(R2)2, NHCOR2; R5R6, R6R7, R7R8 = (CH2)4, CH:CHCH:CH, etc.; R9, R10 = C6H4(R11)m, 2-furyl, cyclohexyl; R11 = H, C1-20-alkyl, C1-20-alkoxy, aryl, aryloxy, SO3Na, COR12, F, Cl, N(R12)2, NHCOR12; R12 = H, C1-20-alkyl; m = 0 - 3] or II [Q = PPh2, P(cyclohexyl)2, P(C6H3(CF3)2-3,5], P(4-methoxy-3,5-dimethylphenyl)2, P(CMe3)2; Y = OH, P(cyclohexyl)2, P(C6H3Me2-3,5)2, P(CMe3)2; Z = H, PPh2; Ph = unsubstituted Ph, C6H4Me-2, C6H4Me-3, C6H4Me-4, C6H3Me2]. Thus, (S)-N-methyl-3-hydroxy-3-(2-thienyl)propanamine was prepared with 92.8% e.e. from 3-(methylamino)-1-(2-thienyl)-1-propanone via asym. hydrogenation in MeOH/PhMe containing catalytic bis(1,5-cyclooctadiene)dirhodium(I) dichloride and (S)-(-)-2,2'-bis[di(p-tolyl)phosphine]-1,1'-binaphthyl.

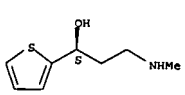
ACCESSION NUMBER: 2004:203795 HCAPLUS
DOCUMENT NUMBER: 140:253262
TITLE: Method for the preparation amino alcohols via the enantioselective hydrogenation of amino ketones

L8 ANSWER 42 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INVENTOR(S): Kralik, Joachim; Fabian, Kai; Muermann, Christoph; Schweickert, Norbert
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004020389	A1	20040311	WO 2003-EP8513	20030801
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2496883	A1	20040311	CA 2003-2496883	20030801
AU 2003260347	A1	20040319	AU 2003-260347	20030801
EP 1532100	A1	20050525	EP 2003-790842	20030801
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003013795	A	20050712	BR 2003-13795	20030801
CN 1678562	A	20051005	CN 2003-820304	20030801
JP 2005536556	T	20051202	JP 2004-531845	20030801
US 2005261514	A1	20051124	US 2005-525821	20050225
ZA 2005002458	A	20051010	ZA 2005-2458	20050324
IN 2005KN00496	A	20060113	IN 2005-KN496	20050324
PRIORITY APPLN. INFO.:			DE 2002-10240025 A	20020827
			WO 2003-DE8513 W	20030801
			WO 2003-EP8513 W	20030801

OTHER SOURCE(S): CASREACT 140:253262; MARPAT 140:253262
IT 116539-55-0P, (S)-3-(Methylamino)-1-(2-thienyl)-1-propanol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation amino alcs. via the enantioselective hydrogenation of amino ketones with chiral diphosphine liganda)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



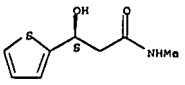
L8 ANSWER 42 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

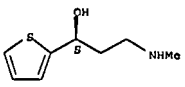
L8 ANSWER 43 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of (3S)-3-oxy-3-(2-thiophen)propylamines and related compds. via an enantioselective Reformatskii reaction)
RN 603959-56-4 HCAPLUS
CN 2-Thiophenepropanamide, β-hydroxy-N-methyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

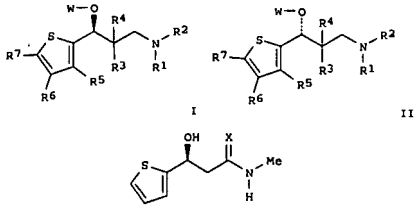


IT 116539-55-0P, N-Methyl-(S)-(-)-3-Hydroxy-3-(2-thiophen)propylamine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (3S)-3-oxy-3-(2-thiophen)propylamines and related compds.
via an enantioselective Reformatskii reaction)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 43 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 11 Mar 2004
GI



I II III

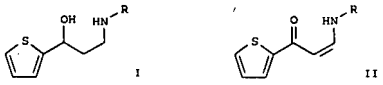
AB Title compds. I and II [R1, R2 = H, halo-alkyl, CN-alkyl; R3, R4, R5, R6, R7 = H, halo, halo-alkyl; W = H, alkyl, acyl, etc.] were prepared via a sparteine mediated enantioselective Reformatskii reaction. For example, LAH reaction of amide II (X = O), e.g., prepared from 2-thiophenecarboxaldehyde in 2-steps, afforded propylamine in 90% yield and 89% ee (HPLC).

ACCESSION NUMBER: 2004:198151 HCAPLUS
DOCUMENT NUMBER: 140:253344
TITLE: Preparation of (3R) - or (3S)-3-oxy-3-(2-thiophen)propylamines and related compounds via an enantioselective Reformatskii reaction
INVENTOR(S): Sorger, Klaus; Stratmann, Oliver; Petersen, Hermann; Stohrer, Juergen
PATENT ASSIGNEE(S): Consortium fuer Elektrochemische Industrie G.m.b.H., Germany
SOURCE: Ger. Offen., 29 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10237272	A1	20040311	DE 2002-10237272	20020814
PRIORITY APPLN. INFO.:			DE 2002-10237272	20020814

OTHER SOURCE(S): MARPAT 140:253344
IT 603959-56-4P, N-Methyl-(S)-(-)-3-Hydroxy-3-(2-thiophen)propionamide

L8 ANSWER 44 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Feb 2004
GI



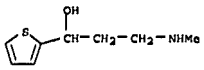
I II

AB This invention pertains to a method for producing N-monoalkyl-3-hydroxy-3-(2-thienyl)propanamines with general formula of I [where R = alkyl], which comprises reduction of II with NaBH4 or Na(CN)H3. For example, β-oxo-β-(2-thienyl)propanal sodium salt was treated with MeNH2 in MeOH, followed by the addition of aqueous NaOH to give (Z)-N-methyl-3-oxo-3-(2-thienyl)-1-propenamine (74.8%). The propenamine was treated with NaBH4 in PhMe in the presence of AcOH to afford the title compound N-methyl-3-hydroxy-3-(2-thienyl)-1-propanamine (75.0%). By the process, an N-monoalkyl-3-hydroxy-3-(2-thienyl)propanamine useful as an intermediate for various medicines can be industrially and easily produced at low cost.

ACCESSION NUMBER: 2004:162681 HCAPLUS
DOCUMENT NUMBER: 140:199199
TITLE: Process for preparation of N-monoalkyl-3-hydroxy-3-(2-thienyl)propanamines
INVENTOR(S): Kogami, Kenji; Hayashizaka, Noriyuki; Satake, Syuzo; Fuseya, Ichiro; Kagano, Hirokazu
PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004016603	A1	20040226	WO 2003-JP8950	20030715
W: CA, CN, JP, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2493776	A1	20040226	CA 2003-2493776	20030715
EP 1541569	A1	20050615	EP 2003-741391	20030715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
CN 1671686	A	20050921	CN 2003-818466	20030715
US 2005240030	A1	20051027	US 2005-523287	20050203
PRIORITY APPLN. INFO.:			JP 2002-229204 A	20020806
			WO 2003-JP8950 W	20030715

L8 ANSWER 44 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 140:199199
IT 116539-56-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of (thienyl)propanamines via reduction reaction)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 45 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 13 Feb 2004
AB A process for the preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol (I) comprises treatment of of a mixture of (R)- and (S)-3-hydroxy-3-thien-2-ylpropionitrile with an acylating agent in the presence of a hydrolase to give a mixture of unacylated (S)-3-hydroxy-3-thien-2-ylpropionitrile and acylated (R)-nitrile and treatment of the former with hydrogen and methylamine in the presence of a catalyst. Thus, 3-hydroxy-3-thien-2-ylpropionitrile (preparation given) was shaken with lipase from Pseudomonas DSM 8246 and vinyl hexanoate in Me tert-Bu ether for 6 h at room temperature to give after flash chromatog. 48% (S)-3-hydroxy-3-thien-2-ylpropionitrile in 99.4% enantiomeric excess. The latter was autoclaved with MeNH2 in MeOH over Raney Ni under 50 bar H2 at 65° for 24 h to give 79% I.
ACCESSION NUMBER: 2004:120843 HCAPLUS
DOCUMENT NUMBER: 140:181317
TITLE: Preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol from racemic 3-hydroxy-3-(thien-2-yl)propionitrile via kinetic resolution with an acylating agent and a lipase followed by treatment with methylamine and hydrogen in the presence of a catalyst.
INVENTOR(S): Stuermer, Rainer
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

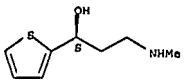
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004013123	A1	20040212	WO 2003-EP8492	20030731
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10235206	A1	20040219	DE 2002-10235206	20020801
CA 2493451	A1	20040212	CA 2003-2493451	20030731
AU 2003251677	A1	20040223	AU 2003-251677	20030731
EP 1527065	A1	20050504	EP 2003-766383	20030731
EP 1527065	B1	20061122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

L8 ANSWER 45 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

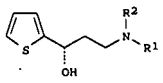
CN 1671687	A	20050921	CN 2003-818510	20030731
JP 2006507234	T	20060302	JP 2004-525403	20030731
AT 346061	T	20061215	AT 2003-766383	20030731
US 2005245749	A1	20051103	US 2005-522888	20050624
PRIORITY APPLN. INFO.:			DE 2002-10235206	A 20020801
			WO 2003-EP8492	W 20030731

OTHER SOURCE(S): CASREACT 140:181317
IT 116539-55-0P, (S)-3-Methylamino-1-(thien-2-yl)propan-1-ol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 46 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 08 Feb 2004
GI



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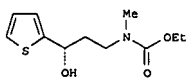


II

AB Title compds. I (wherein R1 and R2 = independently H, (cyclo)alkyl, acyl, alkoxycarbonyl, (hetero)aryl, (hetero)aralkyl, alkylcycloalkyl, alkyl(hetero)aryl; or NR1R2 = (un)substituted heterocyclyl], intermediates for the synthesis of enantiomer-pure bioactive substances, were prepared by catalytic enantioselective hydrogenation of the corresponding α-heteroaryl ketones. Inter alia Ru catalysts with chiral diamine and chiral biphosphine ligands were used. For example, 3-[N-ethoxycarbonyl-N-methylamino]-1-(2-thienyl)-1-propanone was introduced to a Buchi stirred autoclave, which was then evacuated. A mixture of (R)-TolBINAP-RuCl2-(1R,2R)-diphenylethylenediamine and KOBu-t in iPrOH was added. Flushing with H2, pressurizing to 10 bar, and heating to 40° for 2 h provided II in >96% yield with an enantiomeric excess of 80.1%. The content of cyclic carbamate byproduct increased significantly after standing for a fairly long time.
ACCESSION NUMBER: 2004:101154 HCAPLUS
DOCUMENT NUMBER: 140:163699
TITLE: Process for the preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of the corresponding ketones
INVENTOR(S): Hems, William; Rossen, Kai; Reichert, Dietmar; Koehler, Klaus; Almena Perea, Juan Jose
PATENT ASSIGNEE(S): Degussa A.-G., Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011452	A1	20040205	WO 2003-EP7927	20030721
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10233724	A1	20040205	DE 2002-10233724	20020724

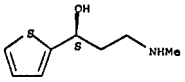
L8 ANSWER 46 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

DE 10258098	A1	20040701	DE 2002-10258098	20021211
CA 2493228	A1	20040205	CA 2003-2493228	20030721
AU 2003258532	A1	20040216	AU 2003-258532	20030721
EP 1523479	A1	20050420	EP 2003-771063	20030721
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671685	A	20050921	CN 2003-817590	20030721
JP 2006502996	T	20060126	JP 2004-523756	20030721
US 2005272930	A1	20051208	US 2005-521799	20050121
IN 2005KN00259	A	20070105	IN 2005-KN259	20050224

PRIORITY APPLN. INFO.: DE 2002-10233724 A 20020724
DE 2002-10258098 A 20021211
WO 2003-EP7927 W 20030721

OTHER SOURCE(S): CASREACT 140:163699; MARPAT 140:163699
IT 116539-55-0P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of corresponding ketones)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 47 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Jan 2004
AB (S)-3-methylamino-1-(2-thienyl)-1-propanol was prepared via fractional crystallization of diastereomeric 3-methylamino-1-(2-thienyl)-1-propanol in the presence of (-)-diacetone-2-keto-L-gulonic acid and subsequent liberation of the free base. Thus, racemic 3-methylamino-1-(2-thienyl)-1-propanol in MeOCMe3 at 50° was treated with a 50° solution of (-)-diacetone-2-keto-L-gulonic acid in EtOH followed by cooling to room temperature, reflux for 3 h, stirring to room temperature over 3 h, and stirring at room temperature for 2 h to give 34.1% (S)-3-methylamino-1-(2-thienyl)-1-propanol (-)-2,3,4,6-di-O-isopropyliden-2-keto-L-gulonic acid salt. This in H2O was treated with 2 equivalent aqueous 6N NaOH followed by extraction with EtOAc to give 97% (S)-3-methylamino-1-(2-thienyl)-1-propanol in 98.4% enantiomeric excess.
ACCESSION NUMBER: 2004:57306 HCAPLUS
DOCUMENT NUMBER: 140:128264
TITLE: Preparation of (S)-3-methylamino-1-(2-thienyl)-1-propanol (-)-2,3,4,6-di-O-isopropyliden-2-keto-L-gulonic acid salt as a means of resolving 3-methylamino-1-(2-thienyl)-1-propanol.
INVENTOR(S): Boehm, Andreas; Sorger, Klas
PATENT ASSIGNEE(S): Consortium fuer Elektrochemische Industrie G.m.b.H., Germany
SOURCE: Ger., 9 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

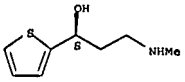
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10237246	B3	20040122	DE 2002-10237246	20020814

PRIORITY APPLN. INFO.: DE 2002-10237246 20020814

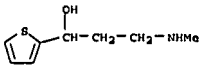
IT 116539-55-0P, (S)-3-Methylamino-1-(2-thienyl)-1-propanol
RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(preparation of (S)-3-methylamino-1-(2-thienyl)-1-propanol (-)-2,3,4,6-di-O-isopropyliden-2-keto-L-gulonic acid salt as a means of resolving 3-methylamino-1-(2-thienyl)-1-propanol)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 47 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 116539-56-1, 3-Methylamino-1-(2-thienyl)-1-propanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (S)-3-methylamino-1-(2-thienyl)-1-propanol (-)-2,3,4,6-di-O-isopropyliden-2-keto-L-gulonic acid salt as a means of resolving 3-methylamino-1-(2-thienyl)-1-propanol)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)

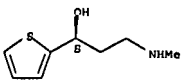


IT 569687-76-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (S)-3-methylamino-1-(2-thienyl)-1-propanol (-)-2,3,4,6-di-O-isopropyliden-2-keto-L-gulonic acid salt as a means of resolving 3-methylamino-1-(2-thienyl)-1-propanol)
RN 569687-76-9 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

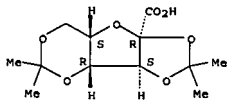
Absolute stereochemistry. Rotation (-).



CM 2

CRN 18467-77-1
CMF C12 H18 O7

L8 ANSWER 47 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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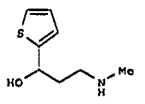
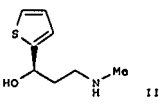
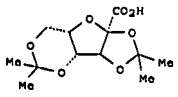
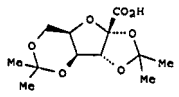
L8 ANSWER 48 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 18 Jan 2004
GI


I


II


III


IV

AB Enantiomerically enriched (S)-(-)-3-N-methylamino-1-(2-thienyl)-1-propanol (I) or (R)-(+)-3-N-methylamino-1-(2-thienyl)-1-propanol (II) or mirror image are prepared by (i) treating an enantiomeric mixture of the amines I and II with (-)-2,3:4,6-di-O-isopropylidene-2-keto-L-gulonic acid (III) or (+)-2,3:4,6-di-O-isopropylidene-2-keto-D-gulonic acid (IV), (ii) crystallizing the obtained diastereomerically enriched salts from the reaction mixture obtained in step (i), (iii) optionally recrystg. said diastereomerically enriched salts I.III or II.IV, and (iv) treating the diastereomerically enriched salts II.III or II.IV obtained in step (ii) or step (iii) with a base to liberate the enantiomerically enriched amines I or II.

ACCESSION NUMBER: 2004:41488 HCAPLUS
DOCUMENT NUMBER: 140:93915
TITLE: Process for the preparation of optically active 3-N-methylamino-1-(2-thienyl)-1-propanol
INVENTOR(S): Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

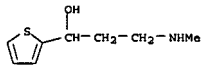
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005307	A1	20040115	WO 2003-EP7312	20030708

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003253036	A1	20040123	AU 2003-253036	20030708
PRIORITY APPLN. INFO.:			EP 2002-15161	A 20020709
			WO 2003-EP7312	W 20030708

OTHER SOURCE(S): CASREACT 140:93915; MARPAT 140:93915
IT 116539-56-1P, (±)-3-(N-Methylamino)-1-(2-thienyl)-1-propanol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of optically active N-methylamino(thienyl)propanol by optical resolution via formation of diastereomer salts with 2,3:4,6-di-O-isopropylidene-2-ketogulonic acid)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)

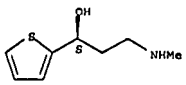


IT 569687-76-9P 645417-43-2P 645417-44-3P
645417-45-4P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active N-methylamino(thienyl)propanol by optical resolution via formation of diastereomer salts with 2,3:4,6-di-O-isopropylidene-2-ketogulonic acid)
RN 569687-76-9 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

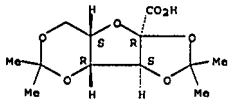
Absolute stereochemistry. Rotation (-).



CM 2

CRN 18467-77-1
CMF C12 H18 O7

Absolute stereochemistry. Rotation (-).

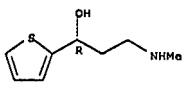


RN 645417-43-2 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αR)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-57-2
CMF C8 H13 N O S

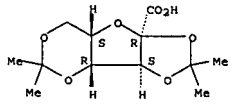
Absolute stereochemistry. Rotation (+).



CM 2

CRN 18467-77-1
CMF C12 H18 O7

Absolute stereochemistry. Rotation (-).

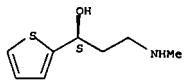


RN 645417-44-3 HCAPLUS
CN α-D-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

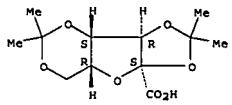
Absolute stereochemistry. Rotation (-).



CM 2

CRN 114559-95-4
CMF C12 H18 O7

Absolute stereochemistry.



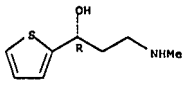
RN 645417-45-4 HCAPLUS
CN α-D-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αR)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-57-2
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (+).

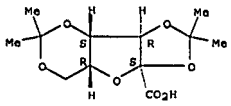
L8 ANSWER 48 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

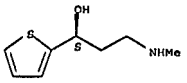
CRN 114559-95-4
CMF C12 H18 O7

Absolute stereochemistry.



IT 116539-55-0P, (S)-(-)-3-(N-Methylamino)-1-(2-thienyl)-1-propanol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active N-methylamino(thienyl)propanol by optical
resolution via formation of diastereomer salts with 2,3:4,6-di-O-isopropylidene-2-ketogulonic acid)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

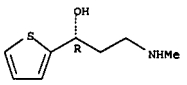
Absolute stereochemistry. Rotation (-).



IT 116539-57-2P, (R)-(+)-3-(N-Methylamino)-1-(2-thienyl)-1-propanol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active N-methylamino(thienyl)propanol by optical
resolution via formation of diastereomer salts with 2,3:4,6-di-O-isopropylidene-2-ketogulonic acid)
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

L8 ANSWER 48 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 49 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 18 Jan 2004
AB The invention relates to a process for the synthesis of N-monosubstituted β-amino alcs. of formula HOCH(R1)CH2CH2NHR2 and/or an addition salt of a proton acid (wherein R1 and R2 independently represent alkyl, cycloalkyl, aryl or aralkyl, each being optionally further substituted with alkyl, alkoxy and/or halogen) via direct preparation of N-monosubstituted β-amino
ketones of R1COCH2CH2NHR2 and its addition salts of proton acids (wherein R1
and R2 are as defined above). Thus, 2-acetylthiophene 26.5, methylamine hydrochloride 14.9, paraformaldehyde 8.2, concentrated HCl 1.0 g, 100 mL ethanol
were heated in an autoclave at 110° and a total pressure of 2-2.5 bar for 9 h, followed by removing 50 mL ethanol in vacuo and addition of 200
mL Et acetate under vigorous stirring, and filtration to give 71% 3-(methylamino)-1-(thiophen-2-yl)propan-1-one hydrochloride (I). To a mixture of 10.3 g I and 35 mL ethanol at 4° sodium hydroxide (4.0 g of a 50% aqueous solution) was added in about 5 min and afterwards, 0.95 g neat
sodium borohydride in several portions in about 30 min. The resulting suspension was stirred for 4 h at the same temperature, treated dropwise with
10.0 mL acetone in 5 min, stirred for 10 addnl. minutes, treated with 20 mL H2O, concentrated about 5 times under vacuum, and extracted with tert-Bu Me ether
(2 x 20 mL). The collected organic phases were finally concentrated under vacuum
affording an orange oil which crystallized spontaneously after a few hours to
give 3-(methylamino)-1-(thiophen-2-yl)propan-1-ol as an orange solid (7.2 g, 84 % yield).
ACCESSION NUMBER: 2004:41430 HCAPLUS
DOCUMENT NUMBER: 140:93914
TITLE: Process for the preparation of N-monosubstituted β-amino alcohols
INVENTOR(S): Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005239	A1	20040115	WO 2003-EP7411	20030709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2491472	A1	20040115	CA 2003-2491472	20030709

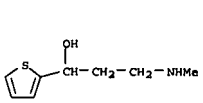
L8 ANSWER 49 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AU 2003250924	A1	20040123	AU 2003-250924	20030709
BR 2003012651	A	20050426	BR 2003-12651	20030709
EP 1539673	A1	20050615	EP 2003-762669	20030709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1665773	A	20050907	CN 2003-816223	20030709
JP 2005532383	T	20051027	JP 2004-518758	20030709
NZ 537567	A	20061130	NZ 2003-537567	20030709
CN 1891683	A	20070110	CN 2006-10100705	20030709
IN 2004CN03142	A	20060217	IN 2004-CN3142	20041231
NO 2005000079	A	20050311	NO 2005-79	20050106
US 2005256318	A1	20051117	US 2005-520362	20050418

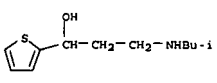
PRIORITY APPLN. INFO.:

EP 2002-15229	A	20020709
CN 2003-816223	A3	20030709
WO 2003-EP7411	W	20030709

OTHER SOURCE(S): CASREACT 140:93914; MARPAT 140:93914
IT 116539-56-1P, 3-(Methylamino)-1-(thiophen-2-yl)propan-1-ol
645411-22-9P, 3-(Isobutylamino)-1-(thiophen-2-yl)propan-1-ol
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for preparation of N-monosubstituted β-amino alcs. by reduction of
N-monosubstituted β-amino ketones)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)

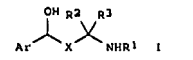


RN 645411-22-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-methylpropyl)amino]ethyl]- (9CI) (CA INDEX NAME)

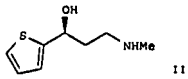


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 50 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 11 Jan 2004
GI



I



II

AB The invention is directed to a process for preparation of an optically active isomer of I by resolution of its racemate with diprogulic acid or a salt of this acid [wherein Ar = heteroaryl; R1 = alkyl; R2, R3 = independently H, alkyl; X = (CH2)n; n = 0-4]. The advantage includes the preparation of desired optically active heteroarylmonoalkylaminoalkanols, in particular (S)-II, well-known intermediate in the synthesis of duloxetine. For example, (S)-II was prepared by resolution of racemic-II with diprogulic acid in 2-propanol, recrystn. from ethanol to give II•diprogulic acid in 91% yield and 95% d.e., followed by hydrolysis. Racemic-II was prepared by acylation of thiophene with propionyl chloride, reduction with NaBH4/EtOH, and alkylation with methylamine.

ACCESSION NUMBER: 2004:19767 HCAPLUS
DOCUMENT NUMBER: 140:77017
TITLE: Process for preparation of an optically active isomer of heteroarylmonoalkylaminoalkanols, in particular (S)-1-(2-Thiophene)-3-methylamino-1-propanol, by resolution of their racemates with diprogulic acid diprogulic acid
INVENTOR(S): Roussisse, Sonia; Frein, Stephane; Burgos, Alain; Bertrand, Blandine; Clementz, Myriam; Total, Avril
PATENT ASSIGNEE(S): PPG-Sipsy, Fr.
SOURCE: Fr. Demande, 16 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2841899	A1	20040109	FR 2002-8516	20020705
WO 2004005220	A2	20040115	WO 2003-FR2086	20030704
WO 2004005220	A3	20040415		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

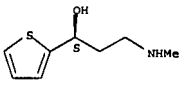
AU 2003263264	A1	20040123	AU 2003-263264	20030704
PRIORITY APPLN. INFO.:			FR 2002-8516 A	20020705
			WO 2003-FR2086 W	20030704

OTHER SOURCE(S): CASREACT 140:77017; MARPAT 140:77017

IT 116539-55-0P
RL: IMF (Industrial manufacture); PREP (Preparation)
(chiral thiophenylalc. product; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)

RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



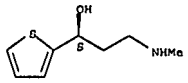
IT 569687-76-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereomeric salt intermediate; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)

RN 569687-76-9 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

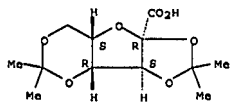
Absolute stereochemistry. Rotation (-).



CM 2

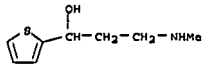
CRN 18467-77-1
CMF C12 H18 O7

Absolute stereochemistry. Rotation (-).



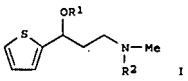
IT 116539-56-1P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for preparation of optically active heteroarylmonoalkylaminoalkanols by resolution of its racemates with diprogulic acid diprogulic acid)

RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 51 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 28 Nov 2003
GI



I

AB A process is provided, by which 3-N-methylamino-1-(2-thienyl)-1-propanols represented by the general formula (I)(wherein R1 is hydrogen, C1-8 acyl, substituted or unsubstituted C1-8 alkyloxycarbonyl, or substituted or unsubstituted phenyloxycarbonyl; and R2 is hydrogen, C1-8 alkyl, substituted or unsubstituted benzyl, C1-8 acyl, substituted or unsubstituted C1-8 alkyloxycarbonyl, or substituted or unsubstituted phenyloxycarbonyl, with the proviso that a case wherein R1 is hydrogen and R2 is Me or hydrogen is excepted) can be easily prepared in the form of a racemate or an optically active substance of S- or R-configuration at a low cost and in a high yield. The compds. I are useful as intermediates for drugs and agrochems., e.g. (S)-enantiomer for duloxetine (antidepressant). Thus, 36.9 g N-benzylmethylamine (0.30 mmol) was dissolved in 40 mL ethanol, treated with 30.0 g 37% aqueous HCl (0.30 mmol) to convert it to the hydrochloride salt, treated with 30 g 2-acetylthiophene, 10.8 g paraformaldehyde, 20 mL ethanol, and 1.2 g 37% aqueous HCl (0.01 mmol), heated at 80° under reflux for 4 h, cooled to room temperature, and filtered, followed by washing the crystals with ethanol and drying under reduced pressure to give 57.7 g 3-(N-benzylmethylamino)-1-(2-thienyl)-1-propanone (II) as the HCl salt. A 0.5 M KOH/2-propanol (40 μL), 2.1 mg (R,R)-1,2-diphenylethylenediamine, 873 mg II, and 3 mL 2-propanol were added to a Schlenk reaction tube, degassed and purged with Ar, treated with 9.6 mg RuCl2[(R)-BINAP](DMF)n, repeatedly degassed and purged with Ar, dissolved completely, transferred to a glass autoclave, pressurized with H, and stirred at 28° for 6 h to give (S)-3-(N-benzylmethylamino)-1-(2-thienyl)-1-propanol (96% ee).

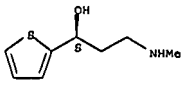
ACCESSION NUMBER: 2003:931354 HCAPLUS
DOCUMENT NUMBER: 139:395802
TITLE: Preparation of propanolamine derivatives, process for preparation of 3-N-methylamino-1-(2-thienyl)-1-propanols, and process for preparation of propanolamine derivatives
INVENTOR(S): Inoue, Yoshiki; Mori, Hiroyuki; Nogami, Hiroyuki; Saitou, Takayuki; Ogura, Kuniyoshi
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

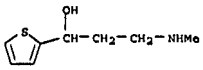
L8 ANSWER 51 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
WO 2003097632 A1 20031127 WO 2003-JP6225 20030519
W: CN, JP, US
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR
EP 1506965 A1 20050216 EP 2003-752916 20030519
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
US 2006167278 A1 20060727 US 2005-513790 20050527
PRIORITY APPLN. INFO.: JP 2002-145394 A 20020520
JP 2001-256621 A 20010827
WO 2003-JP6225 W 20030519

OTHER SOURCE(S): MARPAT 139:395802
IT 116539-55-0P 116539-56-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (methylamino)thienylpropanols)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

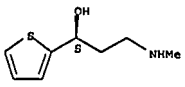


RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



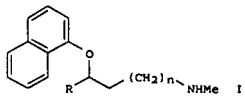
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 52 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

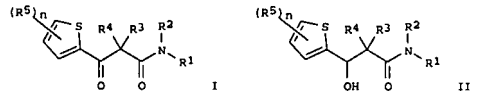
L8 ANSWER 52 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 28 Nov 2003
GI



AB A series of naphthalenyloxy-substituted amines I (n = 2 - 4, R = H; n = 1,
R = H, Ph, 4-FC6H4, 2-MeOC6H4, 2-furyl, 2-thienyl, 2-thiazolyl, etc.) has been prepared, and these compds. are demonstrated to be inhibitors of both
serotonin and norepinephrine reuptake. One member of this series, duloxetine (Cymbalta), (S)-I (n = 1; R = 2-thienyl), has proven to be effective in clin. trials for the treatment of depression.
ACCESSION NUMBER: 2003:928895 HCAPLUS
DOCUMENT NUMBER: 140:145879
TITLE: Duloxetine (Cymbalta), a dual inhibitor of serotonin and norepinephrine reuptake
AUTHOR(S): Bymaster, F. P.; Beedle, E. E.; Findlay, J.; Gallagher, P. T.; Krushinski, J. H.; Mitchell, S.; Robertson, D. W.; Thompson, D. C.; Wallace, L.; Wong, D. T.
CORPORATE SOURCE: Eli Lilly and Company, Lilly Research Laboratories, Lilly Corporate Center, Indianapolis, IN, 46285, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(24), 4477-4480
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:145879
IT 116539-55-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(O-arylation; preparation of naphthalenyloxy-substituted amines as dual
inhibitors of serotonin and norepinephrine reuptake and antidepressive agents)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 53 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 26 Sep 2003
GI



AB This invention pertains to a method for producing 3-oxo-3-(2-thienyl)propionamides with general formula of I [wherein R1 and R2 = independently H, alkyl, aryl, or aralkyl; R3 and R4 = independently H or alkyl; or R3 and R4 together form a ring with the nitrogen atom attached; R5 = halo, NO2, OH, (un)substituted alkyl, aryl, or alkoxy; n = 0-3] and a
process for industrially producing optically active 3-amino-1-(2-thienyl)-
1-propanol derivs. with general formula of II at low cost from the propionamides in high yields with high optical purity. The process compriees subjecting a β-ketocarbonyl compound having a thiophene ring to asym. reduction either in the presence of a catalyst comprising a compound of
a Group 8 or 9 metal of the Periodic Table (e.g., ruthenium compound) and an
asym. ligand (e.g., diphenylethylenediamine derivative) or using cells of a
microorganism. Thus, 2-acetylthiophene was treated with NaH in THF, followed by the addition of di-Et carbonate to give 3-oxo-3-(2-thienyl)propionic acid Et ester (74%). The ester was treated with HCO2H in DMF in the presence of SS-TsDPEN and Et3N to provide (S)-3-hydroxy-3-(2-thienyl)propionic acid Et ester (94%) with 97.5% e.e. The chiral ester was treated with MeNH2 in MeOH to afford (S)-3-hydroxy-N-methyl-3-(2-thienyl)propionamide (93%) with 99% e.e.
ACCESSION NUMBER: 2003:757695 HCAPLUS
DOCUMENT NUMBER: 139:261165
TITLE: Process for preparation of 3-hydroxy-3-(2-thienyl)propionamide derivatives
INVENTOR(S): Takehara, Jun; Qu, Jingping; Kanno, Kazuaki; Kawabata,
Hiroshi; Dekishima, Yasumasa; Ueda, Makoto; Endo, Kyoko; Murakami, Takeshi; Sasaki, Tomoko; Uehara, Hisatoshi; Matsumoto, Youichi; Suzuki, Shihomi
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003078418	A1	20030925	WO 2003-JP3170	20030317

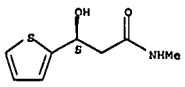
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

L8 ANSWER 53 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

JP 2003335732	A	20031128	JP 2002-141145		20020516
JP 2004067559	A	20040304	JP 2002-227401		20020805
JP 2004067560	A	20040304	JP 2002-227402		20020805
JP 2004067577	A	20040304	JP 2002-228495		20020806
JP 2003342275	A	20031203	JP 2002-317857		20021031
AU 2003221028	A1	20030929	AU 2003-221028		20030317
EP 1486493	A1	20041215	EP 2003-712723		20030317
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2004155756	A	20040603	JP 2003-102914		20030407
US 2005107621	A1	20050519	US 2004-944055		20040920
PRIORITY APPLN. INFO.:			JP 2002-76168	A	20020319
			JP 2002-129140	A	20020430
			JP 2002-141145	A	20020516
			JP 2002-227401	A	20020805
			JP 2002-227402	A	20020805
			JP 2002-228495	A	20020806
			JP 2002-267617	A	20020913
			JP 2002-317857	A	20021031
			WO 2003-JP3170	W	20030317

OTHER SOURCE(S): MARPAT 139:261165
IT 603959-56-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hydroxy(thienyl)propionamide derivs.)
RN 603959-56-4 HCAPLUS
CN 2-Thiophenepropanamide, β-hydroxy-N-methyl-, (βS)- (9CI) (CA INDEX NAME)

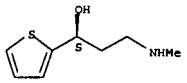
Absolute stereochemistry. Rotation (-).



L8 ANSWER 53 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

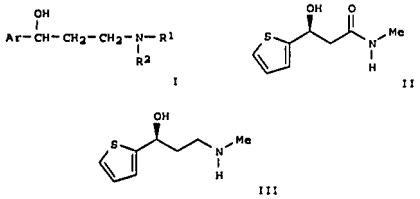
IT 116539-55-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of hydroxy(thienyl)propionamide derivs.)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 54 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 25 Sep 2003
GI



AB Title compds. I [Ar = (un)substituted aryl; R1, R2 = H, alkyl, aryl, etc.] were prepared For example, LAH reduction of amide II, e.g., prepared from 2-acetylthiophene in 3-steps, afforded aminopropanol III in 84% yield. Compds. I are claimed useful intermediates for the production of pharmaceuticals.

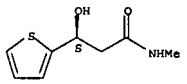
ACCESSION NUMBER:	2003:752682 HCAPLUS
DOCUMENT NUMBER:	139:261162
TITLE:	Preparation of arylaminopropanols via ruthenium mediated enantioselective reduction of β-hydroxy esters
INVENTOR(S):	Eckert, Markus; Dreisbach, Claus; Bosch, Boris; Stolle, Andreas
PATENT ASSIGNEE(S):	Bayer Aktiengesellschaft, Germany
SOURCE:	Eur. Pat. Appl., 24 pp. CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1346977	A1	20030924	EP 2003-4920	20030307
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10212301	A1	20031002	DE 2002-10212301	20020320
US 2003225153	A1	20031204	US 2003-391348	20030318
US 7169938	B2	20070130		
CN 1445224	A	20031001	CN 2003-107316	20030320
JP 2003313184	A	20031106	JP 2003-78367	20030320
PRIORITY APPLN. INFO.:			DE 2002-10212301	A 20020320

OTHER SOURCE(S): CASREACT 139:261162; MARPAT 139:261162
IT 603959-56-4P 603996-86-7P

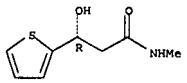
L8 ANSWER 54 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of arylaminopropanols via ruthenium mediated enantioselective redn. of β-hydroxy esters)
RN 603959-56-4 HCAPLUS
CN 2-Thiophenepropanamide, β-hydroxy-N-methyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

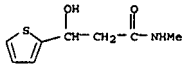


RN 603996-86-7 HCAPLUS
CN 2-Thiophenepropanamide, β-hydroxy-N-methyl-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



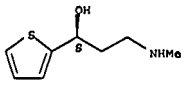
IT 603996-87-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(product; preparation of arylaminopropanols via ruthenium mediated enantioselective reduction of β-hydroxy esters)
RN 603996-87-8 HCAPLUS
CN 2-Thiophenepropanamide, β-hydroxy-N-methyl- (9CI) (CA INDEX NAME)



IT 116539-55-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(product; preparation of arylaminopropanols via ruthenium mediated enantioselective reduction of β-hydroxy esters)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

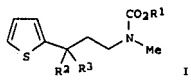
Absolute stereochemistry. Rotation (-).

L8 ANSWER 54 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 55 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Aug 2003
GI



I

AB A novel route is described for the synthesis of N-methyl-3-hydroxy-3-(2-thienyl)propylamine, which can be used as a starting compound for the preparation
of duloxetine. N-Methyl-3-hydroxy-3-(2-thienyl)propylamine is synthesized
via novel thiophene derivs. I [R1 = H, (un)substituted aliphatic, cycloaliph., aromatic; R2R3 = O; R2 = (un)substituted OH, R3 = H]. Thus, 2-acetylthiophene was treated with PhCH2NHMe, followed by ClCO2Et to give I [R1 = Et, R2R3 = O] which was reduced with (R)-Methyl-Corey-Bakshi-Shibata catalyst to give (S)-I [R1 = Et, R2 = OH, R3 = H].

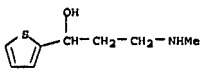
ACCESSION NUMBER: 2003:678803 HCAPLUS
DOCUMENT NUMBER: 139:214324
TITLE: Preparation of N-methyl-3-hydroxy-3-(2-thienyl)propylamine via novel thiophene derivatives containing carbamate groups as intermediates
INVENTOR(S): Reichert, Dietmar; Almena Perea, Juan Jose; Schwarm, Michael; Drauz, Karlheinz; Krimmer, Hans-Peter
PATENT ASSIGNEE(S): Degussa A.-G., Germany
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003070720	A1	20030828	WO 2003-EP910	20030130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR				
DE 10207586	A1	20030911	DE 2002-10207586	20020222
CA 2477082	A1	20030828	CA 2003-2477082	20030130
AU 2003206800	A1	20030909	AU 2003-206800	20030130
EP 1476439	A1	20041117	EP 2003-704496	20030130
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

L8 ANSWER 55 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

JP 2005519077	T	20050630	JP 2003-569627		20030130
US 2005171360	A1	20050804	US 2003-503600		20030130
IN 2004KN01197	A	20060512	IN 2004-KN1197		20040817
PRIORITY APPLN. INFO.:			DE 2002-10207586	A	20020222
			WO 2003-EP910	W	20030130

OTHER SOURCE(S): CASREACT 139:214324; MARPAT 139:214324
IT 116539-56-1P 586968-36-7P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-methyl-3-hydroxy- 3-(2-thienyl)propylamine via novel thiophene derivs. containing carbamate groups as intermediates)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)

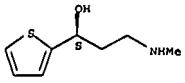


RN 586968-36-7 HCAPLUS
CN Benzeneacetic acid, α-hydroxy-, (αS)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

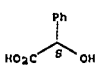
Absolute stereochemistry. Rotation (-).



CM 2

CRN 17199-29-0
CMF C8 H8 O3

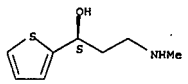
Absolute stereochemistry. Rotation (+).



IT 116539-55-0P 586968-37-8P

L8 ANSWER 55 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of N-methyl-3-hydroxy- 3-(2-thienyl)propylamine via novel thiophene derivs. contg. carbamate groups as intermediates)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

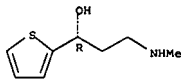


RN 586968-37-8 HCAPLUS
CN Benzeneacetic acid, α-hydroxy-, (αR)-, compd. with (αR)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-57-2
CMF C8 H13 N O S

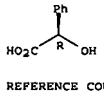
Absolute stereochemistry. Rotation (+).



CM 2

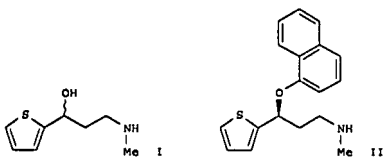
CRN 611-71-2
CMF C8 H8 O3

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 56 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 01 Aug 2003
GI



AB The invention provides an optical resolution process for the synthesis of (S)-3-methylamino-1-(2-thienyl)-1-propanol [(S)-I], a key intermediate in the synthesis of duloxetine (II) and its hydrochloride. The process comprises 3 distinct steps. The first step involves resolution of racemic I using either 2,3,4,6-di-O-isopropylidene-2-keto-L-gulonic acid (III) or (S)-(-)-2-pyrrolidone-5-carboxylic acid as the resolving agent, in a solvent which is preferably iso-PrOH, THF, acetone, or EtOAc, most preferably iso-PrOH. The second step involves racemization of a stereochem. enriched mixture, which may be the undesired isomer (R)-I, and which may be carried out with HCl in iso-PrOH. The third step is a second order asym. induced crystallization of (S)-I, carried out by resolution of racemic I using III as the resolving agent, in a solvent as described above. For instance, a solution of racemic I in iso-PrOH was treated with III, stirred, and filtered to give the diastereomeric salt (S)-I.III in 74% yield and 12% d.e. (diastereomeric excess). Re-suspension of the product salt in iso-PrOH followed by stirring at room temperature and filtration (twice) increased the d.e. to 78% with losses in yield. In a demonstration of the racemization step, I.III with a d.e. of 75% was treated with 1N HCl for 2.5 h and concentrated in vacuo to give a solid showing a d.e. of 32%. In a demonstration of the 3rd step, racemic I and III in iso-PrOH were heated at 40° for 66 h and cooled and filtered to give crystalline (S)-I.III in 76% yield and 76% d.e. Mass balance anal. showed formation of the desired diastereomer at the expense of the unwanted one.

ACCESSION NUMBER: 2003:591163 HCAPLUS
DOCUMENT NUMBER: 139:149519
TITLE: Process for preparing (S)-3-methylamino-1-(2-thienyl)-

L8 ANSWER 56 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

1-propanol, an intermediate useful for the asymmetric synthesis of duloxetine, via optical resolution

INVENTOR(S): Borghese, Alfio
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 12 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003062219	A1	20030731	WO 2003-US18	20030113
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1478641	A1	20041124	EP 2003-707289	20030113
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2004249170	A1	20041209	US 2004-500829	20040707
PRIORITY APPLN. INFO.:			US 2002-351622P	P 20020124
			WO 2003-US18	W 20030113

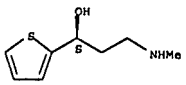
IT 569687-76-9P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereomeric salt; process for preparation of a chiral duloxetine intermediate by optical resolution)
RN 569687-76-9 HCAPLUS
CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).

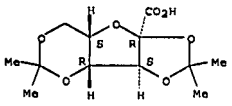
L8 ANSWER 56 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



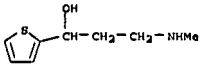
CM 2

CRN 18467-77-1
CMF C12 H18 O7

Absolute stereochemistry. Rotation (-).



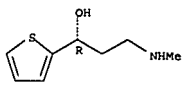
IT 116539-56-1, 3-Methylamino-1-(2-thienyl)-1-propanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(racemic starting material; process for preparation of a chiral duloxetine intermediate by optical resolution)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



IT 116539-57-2P, (R)-3-Methylamino-1-(2-thienyl)-1-propanol
RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(racemization as undesired enantiomer; process for preparation of a chiral duloxetine intermediate by optical resolution)
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

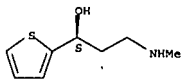
Absolute stereochemistry. Rotation (+).

L8 ANSWER 56 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 116539-55-0P, (S)-3-Methylamino-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(target intermediate; process for preparation of a chiral duloxetine intermediate by optical resolution)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



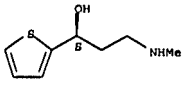
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 57 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 10 Jul 2003
AB (S)-3-N-methylamino-1-(2-thienyl)-1-propanol is prepared by reaction of thiophene with 3-chloropropionyl chloride in the presence of Friedel-Crafts catalysts, hydrogenation of 1-(2-thienyl)-3-chloropropan-1-one (I) in the presence of transition metal-containing asym. hydrogenation catalysts, bases, and optically active N compds., and reaction of (S)-3-chloro-1-(2-thienyl)-1-propanol (II) with MeNH2. I was hydrogenated in 2-propanol in the presence of KOH, (R,R)-diphenylethylenediamine, and RuCl2[(R)-BINAP](DMF)n at 28° for 6 h to give ≥99% II with 97% ee.
ACCESSION NUMBER: 2003:525413 HCAPLUS
DOCUMENT NUMBER: 139:85232
TITLE: Preparation of optically active thienylpropanols
INVENTOR(S): Ogura, Kuniyoshi; Mori, Hiroyuki; Inoue, Yoshiki
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003192681	A	20030709	JP 2001-397944	20011227
PRIORITY APPLN. INFO.:			JP 2001-397944	20011227

IT 116539-55-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active thienylpropanols via asym. hydrogenation of thienylchloropropanone)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 58 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 10 Jun 2003
AB The resolution of racemic 3-(methylamino)-1-(2-thienyl)propan-1-ol (I), a new key intermediate for duloxetine, was studied. The conditions were optimized for an industrial-scale resolution of I by using (S)-mandelic acid as a resolving agent and 2-butanol containing 2 equimolar amts. of water as a solvent. The (S)-I·(S)-mandelic acid diastereomeric salt was crystallized to give pure (S)-I with >99.9% e.e. after liberation of the amine.
The absolute configuration of liberated (-)-I was determined as (S) by x-ray crystallog.
ACCESSION NUMBER: 2003:442717 HCAPLUS
DOCUMENT NUMBER: 139:245839
TITLE: Resolution of 3-(methylamino)-1-(2-thienyl)propan-1-ol, a new key intermediate for duloxetine, with (S)-mandelic acid
AUTHOR(S): Sakai, Kenichi; Sakurai, Rumiko; Yuzawa, Atsushi; Kobayashi, Yuka; Saigo, Kazuhiko
CORPORATE SOURCE: R & D Division, Yamakawa Chemical Industry Co., Ltd, Kitaibaraki, 319-1541, Japan
SOURCE: Tetrahedron: Asymmetry (2003), 14(12), 1631-1636
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:245839
IT 599173-77-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(resolution of 3-(methylamino)-1-(2-thienyl)propan-1-ol, a new key intermediate for duloxetine, with (S)-mandelic acid)
RN 599173-77-0 HCAPLUS
CN Benzeneacetic acid, α-hydroxy-, (αS)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1), monohydrate (9CI) (CA INDEX NAME)

CM 1

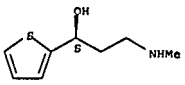
CRN 586968-36-7
CMF C8 H13 N O S . C8 H8 O3

CM 2

CRN 116539-55-0
CMF C8 H13 N O S

Absolute stereochemistry. Rotation (-).

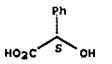
L8 ANSWER 58 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 3

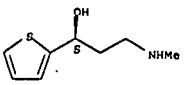
CRN 17199-29-0
CMF C8 H8 O3

Absolute stereochemistry. Rotation (+).

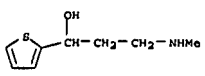


IT 116539-55-0P, (S)-3-(Methylamino)-1-(2-thienyl)propan-1-ol
RL: PUR (Purification or recovery); PREP (Preparation)
(resolution of 3-(methylamino)-1-(2-thienyl)propan-1-ol, a new key intermediate for duloxetine, with (S)-mandelic acid)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



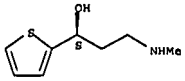
IT 116539-56-1, 3-(Methylamino)-1-(2-thienyl)propan-1-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(resolution of 3-(methylamino)-1-(2-thienyl)propan-1-ol, a new key intermediate for duloxetine, with (S)-mandelic acid)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

L8 ANSWER 59 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 28 May 2003
AB An efficient and facile chemoenzymic synthesis of duloxetine by lipase-mediated resolution of 3-hydroxy-3-(2-thienyl)propanenitrile has been achieved. This process also describes an enantioconvergent synthesis of duloxetine via a Mitsunobu reaction.
ACCESSION NUMBER: 2003:405867 HCAPLUS
DOCUMENT NUMBER: 139:245838
TITLE: Chemoenzymatic synthesis of duloxetine and its enantiomer: lipase-catalyzed resolution of 3-hydroxy-3-(2-thienyl) propanenitrile
AUTHOR(S): Kamal, Ahmed; Khanna, G. B. Ramesh; Ramu, R.; Krishnaji, T.
CORPORATE SOURCE: Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SOURCE: Tetrahedron Letters (2003), 44(25), 4783-4787
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:245838
IT 116539-55-0P 116539-57-2P 597581-29-8P 597581-30-1P
RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(chemoenzymic synthesis of duloxetine and its enantiomers via lipase-catalyzed resolution of hydroxy(thienyl)propanenitrile and its use in enantioconvergent synthesis of duloxetine via Mitsunobu reaction)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

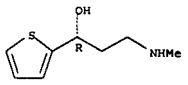
Absolute stereochemistry. Rotation (-).



RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

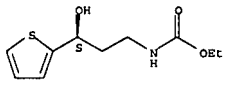
Absolute stereochemistry. Rotation (+).

L8 ANSWER 59 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



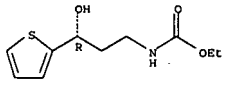
RN 597581-29-8 HCAPLUS
CN Carbamic acid, [(3S)-3-hydroxy-3-(2-thienyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 597581-30-1 HCAPLUS
CN Carbamic acid, [(3R)-3-hydroxy-3-(2-thienyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



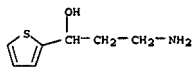
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 60 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 09 May 2003
AB A process for producing an optically active amino alc. is provided that includes a step in which a nitro ketone or a cyano ketone is reacted with a hydrogen-donating organic or inorg. compound in the presence of a transition metal compound catalyst having an optically active nitrogen-containing compound as an asym. ligand to give an optically active nitro alc. or an optically active cyano alc., and a step in which the above optically active alc. is further reduced to efficiently produce an optically active amino alc. Thus, PhCOCH2CN was reduced with HCO2H in presence of Et3N and chloro[(S,S)-N-(p-toluenesulfonyl)-1,2-diphenylethylenediamine](p-cymene)ruthenium to give (S)-HOCHPhCH2CN in 98% ee. This compound was reduced with BH3.Me2S to give (S)-HOCHPhCH2CH2NH2 with 98% ee. The alcs. are intermediates for pharmaceuticals, such as fluoxetine, tomoxetine, nisoxetine and norfluoxetine.
ACCESSION NUMBER: 2003:356091 HCAPLUS
DOCUMENT NUMBER: 138:353733
TITLE: Process for producing optically active amino alcohols
INVENTOR(S): Watanabe, Masahito; Murata, Kunihiko; Ikariya, Takao
PATENT ASSIGNEE(S): Kanto Kagaku Kabushiki Kaisha, Japan
SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

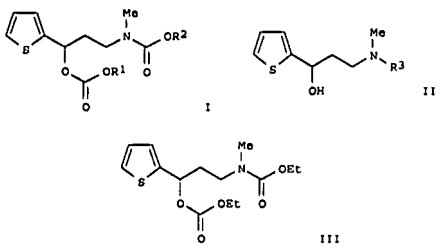
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1308435	A2	20030507	EP 2002-24517	20021030
EP 1308435	A3	20030604		
EP 1308435	B1	20051228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2003201269	A	20030718	JP 2002-251994	20020829
JP 3504254	B2	20040308		
CA 2409906	A1	20030430	CA 2002-2409906	20021028
JP 2003201270	A	20030718	JP 2002-316217	20021030
US 2003171592	A1	20030911	US 2002-285164	20021031
US 6686505	B2	20040203		
PRIORITY APPLN. INFO.:			JP 2001-335322 A	20011031
			JP 2002-251994 A	20020829

OTHER SOURCE(S): MARPAT 138:353733
IT 65653-31-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active amino alcs. via asym. reduction of keto nitriles)
RN 65653-31-8 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 60 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 61 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 07 Mar 2003
GI



I

II

III

AB This invention pertains to prepn method of novel optically active 3-amino-2-thienylpropan-1-ol derivs. with general formula of I and II [wherein R1 and R2 = independently (un)substituted alkyl, alkoxy, alkenyl, alkynyl, (hetero)aralkyl, or (hetero)aryl; R3 = H or CO2R2]. Reaction of optically active 3-(N,N-dimethylamino)-1-(2-thienyl)propan-1-ol with a haloformic ester in the presence of a base provides I. Hydrolysis of I affords alc. II. For example, (S)-3-(N,N-dimethylamino)-1-(2-thienyl)propan-1-ol (96.2% e.e.) was treated with Et chloroformate in PhMe in the presence of NaHCO3 to give III (89%). Compound III was hydrolyzed with NaOH in EtOH and H2O to afford (S)-(2-thienyl)CH(OH)CH2CH2NHMe (80%) with 95.8% e.e.

ACCESSION NUMBER: 2003:173596 HCAPLUS
DOCUMENT NUMBER: 138:221463
TITLE: Process for preparation of 3-(N-alkoxycarbonyl-N-methyl)amino-2-thienylpropan-1-ol derivatives
INVENTOR(S): Ikunaka, Masaya; Matsumoto, Jun; Inoue, Toru
PATENT ASSIGNEE(S): Nagase and Co., Ltd., Japan
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003018572	A1	20030306	WO 2002-JP8588	20020826

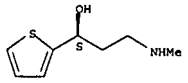
L8 ANSWER 61 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

JP 2005053781	A	20050303	JP 2001-256621	20010827
AU 2002328555	A1	20030310	AU 2002-328555	20020826
PRIORITY APPLN. INFO.:			JP 2001-256621	A 20010827
			WO 2002-JP8588	W 20020826

OTHER SOURCE(S): MARPAT 138:221463
IT 116539-55-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active [(alkoxycarbonyl)methylamino]thienylpropano l derivs.)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

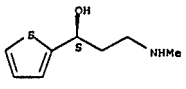


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 62 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 20 Feb 2003
AB Enantioselective hydrogenation using chiral complexes between atropisomeric diphosphines and ruthenium is a powerful tool for producing chiral compds. Using a simple and straightforward in situ catalyst preparation, the conditions were optimized using mol. hydrogen. This led to the best conditions and the lowest catalytic ratio required for the pressure used. Hydrogenation of various β-keto esters was efficiently performed at atmospheric and higher pressures, leading to the use of very low catalyst-substrate ratios up to 1/20,000. Asym. hydrogenations were used in key-steps towards the total synthesis of corynomycolic acid, Duloxetine and Fluoxetine.

ACCESSION NUMBER: 2003:129914 HCAPLUS
DOCUMENT NUMBER: 139:84781
TITLE: Enantioselective hydrogenation of β-keto esters using chiral diphosphine-ruthenium complexes: Optimization for academic and industrial purposes and synthetic applications
AUTHOR(S): Ratovelomanana-Vidal, V.; Girard, C.; Touati, R.; Tranchier, J. P.; Ben Hassine, B.; Genet, J. P.
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels (UMR 7573 CNRS), Ecole Nationale Superieure de Chimie de Paris, Paris, 75005, Fr.
SOURCE: Advanced Synthesis & Catalysis (2003), 345(1+2), 261-274
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:84781
IT 116539-55-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective hydrogenation of β-keto esters using chiral diphosphine-ruthenium complexes)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

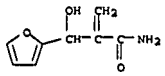


REFERENCE COUNT: 119 THERE ARE 119 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 63 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 08 Jan 2003
AB The reactivity of a variety of quinuclidine-based catalysts in the Baylis-Hillman reaction has been examined, and a straightforward correlation between the basicity of the base and reactivity has been established, without exception. The following order of reactivity was established with pKa's of the conjugate acids (measured in water) given in parentheses: quinuclidine (11.3), 3-hydroxyquinuclidine (9.9), DABCO (8.7), 3-acetoxyquinuclidine (9.3), 3-chloroquinuclidine (8.9), and quinuclidinone (7.2). The higher than expected reactivity of DABCO, based on its pKa, was analyzed by comparing the relative basicity of DABCO and 3-acetoxyquinuclidine in DMSO. It was found that in aprotic solvent, DABCO was 0.6 pKa units more basic than 3-acetoxyquinuclidine, thus establishing a direct link between pKa of the amine and its reactivity. In contrast to previous literature work that reported the contrary, quinuclidine, which has the highest pKa, was found to be the most active catalyst. The reaction profile with quinuclidine showed significant autocatalysis, which suggested that the presence of proton donors might further enhance rates. Thus, a series of additives bearing polar X-H bonds were investigated and it was found that methanol, triethanolamine, formamide, and water all provided addnl. acceleration. Methanol was found to be optimum, and the powerful combination of quinuclidine with methanol was tested with a host of aldehydes and Michael acceptors. Not only were the reactions more efficient and faster than previously reported, but now new substrates that were previously unreactive could be employed. Notable examples include the use of acetylenic aldehydes and the employment of vinyl sulfones, acrylamides, δ-lactones, and even α,β-unsatd. esters bearing a β-substituent.

ACCESSION NUMBER: 2003:13465 HCAPLUS
DOCUMENT NUMBER: 138:169705
TITLE: Correlation between pKa and Reactivity of Quinuclidine-Based Catalysts in the Baylis-Hillman Reaction: Discovery of Quinuclidine as Optimum Catalyst Leading to Substantial Enhancement of Scope
AUTHOR(S): Aggarwal, Varinder K.; Emme, Ingo; Fulford, Sarah Y.
CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK
SOURCE: Journal of Organic Chemistry (2003), 68(3), 692-700
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:169705
IT 497221-43-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(correlation between pKa and reactivity of quinuclidine-based catalysts in the Baylis-Hillman reaction of aldehydes with Michael acceptors)
RN 497221-43-9 HCAPLUS
CN 2-Furanpropanamide, β-hydroxy-α-methylene- (9CI) (CA INDEX NAME)

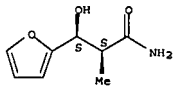
L8 ANSWER 63 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

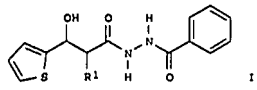
L8 ANSWER 64 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Oct 2002
AB Acid chlorides readily condensed with N-silylated imines in the presence of a base to generate 2-azadienes. These underwent Diels-Alder cycloaddns. with a wide variety of aldehydes. In most cases the cycloaddns. were diastereoselective in favor of the 3,4-cis-oxazinone adducts. Ethanolysis stereoselectively yielded products of hydroxyalkylation or hydroxycarboxylation of the primary amides derived from the initial acid chlorides.
ACCESSION NUMBER: 2002:806270 HCAPLUS
DOCUMENT NUMBER: 138:204491
TITLE: Diastereoselective β-hydroxyalkylation and β-hydroxycarboxylation of amides by a Diels-Alder strategy
AUTHOR(S): Ntirampebura, Deogratias; Ghosez, Leon
CORPORATE SOURCE: Department of Chemistry, Catholic University of Louvain, Louvain-la-Neuve, 1348, Belg.
SOURCE: Synthesis (2002), (14), 2043-2052
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:204491
IT 500166-41-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective Diels-Alder cycloaddn. of azadienes with aldehydes and
subsequent ethanolysis of the oxazinone adducts)
RN 500166-41-6 HCAPLUS
CN 2-Furanpropanamide, β-hydroxy-α-methyl-, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 65 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 28 Feb 2002
GI



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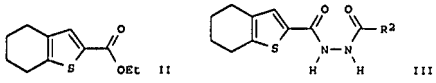
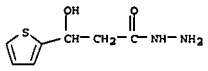


II III

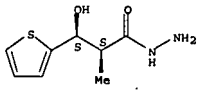
AB Five novel N-benzoyl (thienyl)hydroxypropyl hydrazides I (R1 = H, Me, Et), both erythro- and threo-diastereomers, were synthesized by benzoylation of the corresponding hydrazides under Schotten-Baumann conditions in 61-82% yields. Vilsmeier formylation of cyclohexanone gave 2-chloro-1-cyclohexenecarboxaldehyde, which underwent heterocyclization with Et thioglycolate to afford tetrahydrobenzo[b]thiophene II in 62% yield. Hydrazinolysis of II followed by acylation of the hydrazide with benzoyl chloride or acetic anhydride gave novel N,N'-diacylhydrazines III (R2 = Me, Ph).
ACCESSION NUMBER: 2002:151765 HCAPLUS
DOCUMENT NUMBER: 137:352846
TITLE: Synthesis of thiophene-containing N,N'-diacylhydrazines as potential bioactive compounds
AUTHOR(S): Mavrova, A.; Vasselinova, D.
CORPORATE SOURCE: Dep. Org. Synthesis, Univ. Chem. Technol. Metall., Bulg.
SOURCE: Farmatsiya (Sofia, Bulgaria) (2000), 47(3-4), 7-10
CODEN: FMTYA2; ISSN: 0428-0296
PUBLISHER: Tsentur za Informatsiya po Meditsina
DOCUMENT TYPE: Journal
LANGUAGE: Bulgarian
OTHER SOURCE(S): CASREACT 137:352846
IT 20795-13-5 474900-73-7 474900-75-9 474900-77-1 474900-79-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiophene-containing N,N'-diacylhydrazines via benzoylation of (thienyl)hydroxypropyl hydrazides)
RN 20795-13-5 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-, hydrazide (9CI) (CA INDEX NAME)

L8 ANSWER 65 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



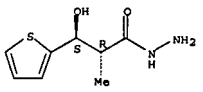
RN 474900-73-7 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, hydrazide, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



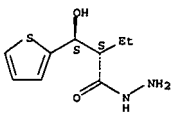
RN 474900-75-9 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, hydrazide, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 474900-77-1 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, hydrazide, (αR,βR)-rel- (9CI) (CA INDEX NAME)

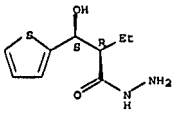
Relative stereochemistry.



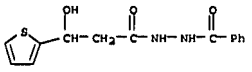
RN 474900-79-3 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, hydrazide, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 65 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

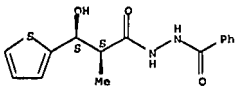


IT 474900-81-7P 474900-83-9P 474900-85-1P
474900-87-3P 474900-89-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of thiophene-containing N,N'-diacylhydrazines via benzoylation of
(thienyl)hydroxypropyl hydrazides)
RN 474900-81-7 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-, 2-benzoylhydrazide (9CI) (CA INDEX NAME)



RN 474900-83-9 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, 2-benzoylhydrazide, (αR,βR)-rel- (9CI) (CA INDEX NAME)

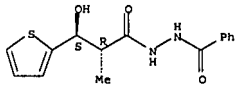
Relative stereochemistry.



RN 474900-85-1 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, 2-benzoylhydrazide, (αR,βS)-rel- (9CI) (CA INDEX NAME)

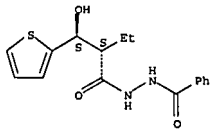
Relative stereochemistry.

L8 ANSWER 65 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



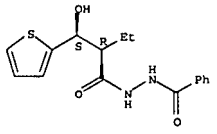
RN 474900-87-3 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, 2-benzoylhydrazide, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

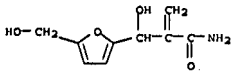


RN 474900-89-5 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, 2-benzoylhydrazide, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

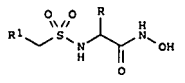


L8 ANSWER 66 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 07 Dec 2001
AB Acrylamide and aromatic aldehydes were found to undergo the Baylis-Hillman
reaction at ambient temperature in an aqueous medium in the presence of a stoichiometric amount of base catalyst, DABCO, to give the corresponding 3-hydroxy-2-methylenepropionamides in 61-99% yield. A faster competing, but reversible, non-Baylis-Hillman reaction was initially observed under the
conditions to form N-acylhemiaminals, which later disappeared, as the desired Baylis-Hillman adduct was formed as the major product over an extended period of time (12-48 h). This represents the first demonstration of the Baylis-Hillman reaction of aldehydes with acrylamides, which were thought to be inert under atmospheric pressure and at
ambient temperature
ACCESSION NUMBER: 2001:878340 HCAPLUS
DOCUMENT NUMBER: 136:134323
TITLE: Successful Baylis-Hillman Reaction of Acrylamide with Aromatic Aldehydes
AUTHOR(S): Yu, Chengzhi; Hu, Longqin
CORPORATE SOURCE: Department of Pharmaceutical Chemistry College of Pharmacy, Rutgers the State University of New Jersey, Piscataway, NJ, 08854-8020, USA
SOURCE: Journal of Organic Chemistry (2002), 67(1), 219-223
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:134323
IT 393561-67-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Baylis-Hillman reaction of acrylamide with aromatic aldehydes)
RN 393561-67-6 HCAPLUS
CN 2-Furanpropanamide, β-hydroxy-5-(hydroxymethyl)-α-methylene- (9CI) (CA INDEX NAME)

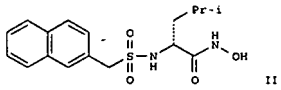


REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 67 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 06 Jul 2001
GI



I



II

AB Compds. I [R = H, alk(en/yn)yl, (hetero)aryl or heterocyclyl; R1 = (hetero)bicyclyl] were prepared. Seventy-five synthetic examples were provided. For instance, sulfonylation of (R)-2-amino-4-methylpentanoic acid tert-Bu ester with naphthalen-2-ylmethanesulfonyl chloride was followed by conversion to hydroxamic acid II. In some instances, the heteroarylmethylsulfonyl chloride was synthesized from the tetra-n-butylammonium sulfonate. I inhibit the formation of s-CD23, IC50 ≤ 1 μM and collagenase, IC50 for selected examples ≥ 10 μM. I are used for the treatment and prophylaxis of conditions mediated by s-CD23 or TNF.
ACCESSION NUMBER: 2001:489359 HCAPLUS
DOCUMENT NUMBER: 135:92375
TITLE: Synthesis of arylmethylsulfonamido hydroxamic acids and their use in treatment of s-CD23 and TNF mediated conditions
INVENTOR(S): Bruton, Gordon; Faller, Andrew; Orlek, Barry Sidney; Rana, Kishore K.; Walker, Graham
PATENT ASSIGNEE(S): Smithkline Beecham P.L.C., UK
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001047874	A1	20010705	WO 2000-GB4941	20001221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

L8 ANSWER 67 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

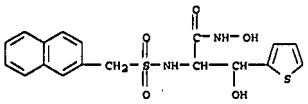
EP 1244616	A1	20021002	EP 2000-985668	20001221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003519119	T	20030617	JP 2001-549347	20001221
US 2003199571	A1	20031023	US 2003-168461	20030324
US 2004225006	A1	20041111	US 2004-846286	20040514
PRIORITY APPLN. INFO.:			GB 1999-30687	A 19991224
			GB 2000-26693	A 20001101
			WO 2000-GB4941	W 20001221
			US 2003-168461	B1 20030324

OTHER SOURCE(S): MARPAT 135:92375

IT 348080-14-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of arylmethylsulfonamido hydroxamic acids and their use in treatment of s-CD23 and TNF mediated conditions)

RN 348080-14-8 HCAPLUS

CN 2-Thiophenepropanamide, N,β-dihydroxy-α-[[(2-naphthalenylmethyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 68 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 01 Jun 2001

AB A method for the removal of a substance, which has a neg. charge and which and which is present in an aqueous liquid (I). The method comprises the steps of: (i) contacting the liquid with an anion-exchanger (1) that comprises mixed mode anion-exchanging ligands in which there is a pos. charged nitrogen allowing binding of the substance to the anion-exchanger; and (ii) desorbing said substance from said anion-exchanger. The characteristic feature is that (A) the mixed mode ligands have a thioether linkage within a distance of 1-7 atoms from their pos. charged atom, and (B) the anion-exchanger (1) (i) is capable of binding the substance of interest in an aqueous reference liquid (II) at an ionic strength corresponding to 0.25 M NaCl, and (ii) permits in the pH interval 2-12 a maximal breakthrough capacity for the substance which is ≥200 of the breakthrough capacity of the substance for Q-Sepharose Fast Flow (anion-exchanger 2).

ACCESSION NUMBER: 2001:396780 HCAPLUS
DOCUMENT NUMBER: 135:10397
TITLE: A method for anion-exchange adsorption and thioether anion-exchangers
INVENTOR(S): Belew, Makonnen; Johansson, Bo-lennart; Maloisel, Jean-luc
PATENT ASSIGNEE(S): Amersham Pharmacia Biotech Ab, Swed.
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001038228	A1	20010531	WO 2000-EP11606	20001122
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2392200	A1	20010531	CA 2000-2392200	20001122
EP 1235749	A1	20020904	EP 2000-988740	20001122
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003531713	T	20031028	JP 2001-539792	20001122
AU 780286	B2	20050310	AU 2001-25079	20001122
PRIORITY APPLN. INFO.:			SE 1999-4197	A 19991122
			WO 2000-EP11606	W 20001122

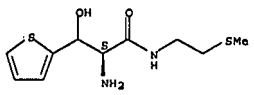
L8 ANSWER 68 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 341014-78-6
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(elution conductivity for three proteins and breakthrough capacity of BSA on Sepharose 6 Fast Flow anion-exchangers modified with ligands containing thioether groups of)

RN 341014-78-6 HCAPLUS

CN 2-Thiophenepropanamide, α-amino-β-hydroxy-N-[2-(methylthio)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 69 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 01 Jun 2001

AB A method for the removal of a substance carrying a neg. charge and being present in an aqueous liquid (I). The method comprises the steps of: (i) contacting the liquid with a matrix carrying a plurality of ligands comprising a pos. charged structure and a hydrophobic structure, and (ii) desorbing the substance. The characterizing feature is that (I) each of said ligands together with a spacer has the formula: -- SP---[Ar-R1-N+(R2R3R4)] where (A) [Ar-R1-N+(R2R3R4)] represents a ligand (a) Ar is an aromatic ring, (b) R1 is [(L)nR'1]m where n and m are integers selected amongst zero or 1; L is amino nitrogen, ether oxygen or thioether sulfur; R'1 is a linker selected among (1) hydrocarbon groups; (2) -C(=NH)-; (c) R2-4 are selected among hydrogen and alkyls; (B) SP is a spacer providing a carbon or a heteroatom directly attached to Ar-R1-N+(R2R3R4); (C) --- represents that SP replaces a hydrogen in [Ar-R1-N+(R2R3R4)]; (D) -- represents binding to the matrix; and (II) desorption. There is also described (a) anion-exchangers having high breakthrough capacities, (b) a screening method and (c) a desalting protocol.

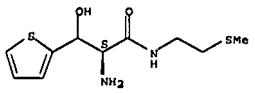
ACCESSION NUMBER: 2001:396779 HCAPLUS
DOCUMENT NUMBER: 135:10396
TITLE: A method for anion-exchange adsorption and anion-exchangers
INVENTOR(S): Johansson, Bo-lennart; Andersson, Mikael; Gustavsson, Jan; Belew, Makonnen; Maloisel, Jean-luc
PATENT ASSIGNEE(S): Amersham Pharmacia Biotech Ab, Swed.
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001038227	A2	20010531	WO 2000-EP11605	20001122
WO 2001038227	A3	20011115		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2389515	A1	20010531	CA 2000-2389515	20001122
EP 1235748	A2	20020904	EP 2000-979615	20001122
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003514664	T	20030422	JP 2001-539791	20001122
AU 782945	B2	20050908	AU 2001-17044	20001122
IL 149783	A	20051120	IL 2000-149783	20001122
US 6702943	B1	20040309	US 2002-130958	20020916
US 2004079702	A1	20040429	US 2003-723362	20031126
PRIORITY APPLN. INFO.:			SE 1999-4197	A 19991122
			WO 2000-EP11605	W 20001122

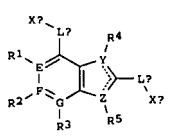
L8 ANSWER 69 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
US 2002-130958 A3 20020916

IT 341014-78-6
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(elution conductivity for three proteins and breakthrough capacity of BSA on
Sepharose 6 Fast Flow anion-exchangers modified with ligands of)
RN 341014-78-6 HCAPLUS
CN 2-Thiophenepropanamide, α-amino-β-hydroxy-N-[2-(methylthio)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 70 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 17 May 2001
GI



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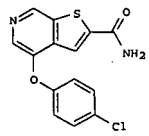


II

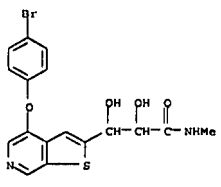
AB The title compds. [I; E, F, and G = C, N, N(:O); Y, Z = C, N, O, S(O)n; n = 0-2; LA = covalent bond, O, S(O)n, etc.; XA = halo, (un)substituted alkyl, etc.; LB = covalent bond, O, S(O)n, etc.; XB = H, alkyl, alkenyl, etc.; R1-R5 = absent, H, halo, etc.] were prepared as antiinflammatory compds. I inhibited the expression of e-selectin and ICAM-1 relative to VCAM-1 and are useful for the treatment or prophylaxis of diseases caused by expression of adhesion mols. Examples include syntheses for over 300 invention compds. and e-selectin, ICAM-1, and VCAM-1 inhibition potencies for approx. 90 representative compds. For instance, 4-chlorophenol was treated with KOBu-t in THF and added to 3,5-dichloropyridine-4-carboxaldehyde in THF. Cycloaddn. with Me thioglycolate in the presence of Cs2CO3, followed by conversion to the amide by heating to 45°C in methanolic NH3 for 18 h, afforded 4-(4-chlorophenoxy)thieno[2,3-c]pyridine-2-carboxamide (II). II inhibited e-selectin, ICAM-1, and VCAM-1 by 82%, 74%, and 50%, resp., at concns. of 1 μM.
ACCESSION NUMBER: 2001:355084 HCAPLUS
DOCUMENT NUMBER: 134:353297
TITLE: Preparation of thienopyridines and thienopyrimidines as cell adhesion-inhibiting antiinflammatory compounds
INVENTOR(S): Stewart, Andrew O.; Boyd, Steven A.; Arendsen, David L.; Bhatia, Pramila; Condroski, Kevin R.; Freeman, Jennifer C.; Gunawardana, Indrani W.; Zhu, Gui-dong; Lartey, Kraig; Mccarty, Catherine M.; Mort, Nicholas A.; Patel, Meena V.; Staeger, Michael A.; Stout, David M.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S., 117 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6232320	B1	20010515	US 1999-325336	19990603
CA 2390948	A1	20001214	CA 1999-2390948	19990628

L8 ANSWER 70 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

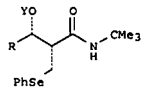
JP 2004509059	T	20040325	JP 2001-502427		19990628
BR 9916746	A	20050111	BR 1999-16746		19990628
US 2001020030	A1	20010906	US 2001-799729		20010306
US 6579883	B2	20030617			
US 2003220365	A1	20031127	US 2003-387317		20030312
PRIORITY APPLN. INFO.:			US 1998-87907P	P	19980604
			US 1999-325336	A	19990603
			WO 1999-US14596	W	19990628
			US 2001-799729	A3	20010306

OTHER SOURCE(S): MARPAT 134:353297
IT 251995-08-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thienopyridines and thienopyrimidines antiinflammatory agents by cycloaddn. of thioglycolates or thiols with halopyridines or halopyrimidines)
RN 251995-08-1 HCAPLUS
CN Thieno[2,3-c]pyridine-2-propanamide, 4-(4-bromophenoxy)-α,β-dihydroxy-N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 71 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 19 Dec 2000
GI



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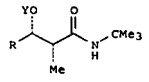
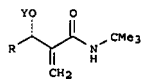
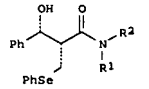


II



III

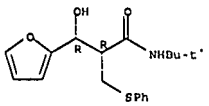


IV

AB The thiolate- or selenolate-induced Michael-aldol tandem process using secondary α,β-unsatd. amides gave α-phenylthio- or α-phenylseleno-methyl-β-hydroxy amides syn-selectively, which were readily converted into NH-amide aldols or Baylis-Hillman adducts. Thus, reacting H2C:CHCONHCMe3 with PhSeSePh and RCHO (R = Ph, 4-ClC6H4, 4-MeOC6H4, 2-furyl) gave hydroxy amides I (Y = H, SiMe2CMe3). I were then
treated with Bu3SnH/AIBN/PhMe at reflux or H2O2/THF at 0°C to give NH-amide aldols II or Baylis-Hillman adducts III, resp. The crystal structure of adducts IV (R1 = CMe3, R2 = H; R1 = R2 = CHMe2) were determined
ACCESSION NUMBER: 2000:887427 HCAPLUS
DOCUMENT NUMBER: 134:237207
TITLE: A simple preparation of syn-NH-amide aldols and amide-Baylis-Hillman adducts via a Michael-aldol tandem process
AUTHOR(S): Kamimura, Akio; Omata, Yoji; Mitsudera, Hiromasa; Kakehi, Akikazu
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Yamaguchi University, Ube, 755-8611, Japan
SOURCE: Perkin 1 (2000), (24), 4499-4504
CODEN: PERKF9; ISSN: 1470-4358
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:237207
IT 329927-28-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(tandem thiolate- and selenolate-induced Michael-aldol of amides with aldehydes and crystal structure of amide-aldol product)
RN 329927-28-8 HCAPLUS
CN 2-Furanpropanamide, N-(1,1-dimethylethyl)-β-hydroxy-α-[(phenylthio)methyl]-, (αR,βR)-rel- (9CI) (CA INDEX NAME)

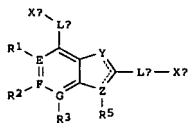
Relative stereochemistry.

L8 ANSWER 71 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

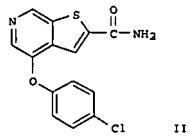


REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 72 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 15 Dec 2000
GI



I



II

AB The title compds. (I) [wherein E, F, and G = independently C, N, or N(:O);
Y and Z = independently C, N, O, or S(O)n; n = 0-2; LA = covalent bond, O,
S(O)n, NR6, C(:W), or alkenylene; R6 = H or (un)substituted alkyl; W = O or S; XA = halo or (un)substituted alkyl; LB = covalent bond, O, S(O)n, NR6, C(:W), or C(:NR13); NR13 = H, NO2, CN, OH, aryloxy, or (un)substituted alkoxy; XB = H, alkoxy, OH, aryl, heterocyclyl, CN, CHO, halo or (un)substituted alkyl, alkenyl, amino, urea, (thio)amido, or B(OH)2; R1-R5 = absent or independently H, halo, alkoxy, perfluoroalkyl, OH, SH, alkylthio, heterocyclyl, or (un)substituted alkyl, carboxy, amido,
arylthio, or amino] were prepared as antiinflammatory compds. I inhibited
the expression of e-selectin and ICAM-1 relative to VCAM-1 and are useful for the treatment or prophylaxis of diseases caused by expression of adhesion mols. Examples include syntheses for over 300 invention compds. and E-selectin, ICAM-1, and VCAM-1 inhibition potencies for approx. 90 representative compds. For instance, 4-chlorophenol was treated with KOBu-t in THF and added to 3,5-dichloropyridine-4-carboxaldehyde in THF. Cycloaddn. with Me thioglycolate in the presence of Cs2CO3, followed by conversion to the amide by heating to 45°C in methanolic NH3 for 18 h, afforded 4-(4-chlorophenoxy)thieno[2,3-c]pyridine-2-carboxamide (II). II inhibited e-selectin, ICAM-1, and VCAM-1 by 82%, 74%, and 50%, resp., at concns. of 1 μM.

ACCESSION NUMBER: 2000:881155 HCAPLUS
DOCUMENT NUMBER: 134:42120
TITLE: Preparation of thienopyridines and thienopyrimidines as cell adhesion-inhibiting antiinflammatory compounds
INVENTOR(S): Arendsen, David L.; Bhatia, Pramila; Boyd, Steven A.; Condroski, Kevin R.; Freeman, Jennifer C.; Gunawardana, Indrani W.; Lartey, Kraig; McCarty, Catherine M.; Mort, Nicholas A.; Patel, Meena V.; Staeger, Michael A.; Stewart, Andrew O.; Stout, David M.; Zhu, Gui-Dong
PATENT ASSIGNEE(S): Abbott Laboratories, USA

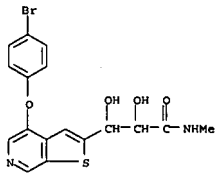
L8 ANSWER 72 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
SOURCE: PCT Int. Appl., 320 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000075145	A1	20001214	WO 1999-US14596	19990628
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2390948	A1	20001214	CA 1999-2390948	19990628
AU 9948388	A1	20001228	AU 1999-48388	19990628
EP 1181296	A1	20020227	EP 1999-931986	19990628
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2004509059	T	20040325	JP 2001-502427	19990628
BR 9916746	A	20050111	BR 1999-16746	19990628

PRIORITY APPLN. INFO.: US 1999-306199 A 19990603
US 1999-325336 A 19990603
WO 1999-US14596 W 19990628

OTHER SOURCE(S): MARPAT 134:42120
IT 251995-08-1P, 3-[4-(4-Bromophenoxy)thieno[2,3-c]pyridin-2-yl]-2,3-dihydroxy-N-methylpropanamide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thienopyridines and thienopyrimidines antiinflammatory agents by cycloaddn. of thioglycolates or thiols with halopyridines or halopyrimidines)
RN 251995-08-1 HCAPLUS
CN Thieno[2,3-c]pyridine-2-propanamide, 4-(4-bromophenoxy)-α,β-dihydroxy-N-methyl- (9CI) (CA INDEX NAME)

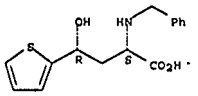
L8 ANSWER 72 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

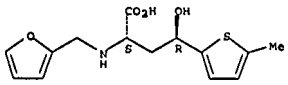
L8 ANSWER 73 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 13 Jul 2000
AB A highly stereoselective reduction of γ-oxo-α-amino acids by sodium borohydride in the presence of a catalytic amount of manganese(II) chloride gives syn-γ-hydroxy-α-amino acids. Enantiomerically pure syn-(2S,4R,1'S)-4-aryl-4-hydroxy-2-(1'-phenylethylamino)butanoic acids form stable gels in methanol.
ACCESSION NUMBER: 2000:471573 HCAPLUS
DOCUMENT NUMBER: 133:238268
TITLE: Stereoselective sodium borohydride reduction, catalyzed by manganese(II) chloride, of γ-oxo-α-amino acids. A practical approach to syn-γ-hydroxy-α-amino acids
AUTHOR(S): Berkes, Dusan; Kolarovic, Andrej; Povazanec, Frantisek
CORPORATE SOURCE: Department of Organic Chemistry, Slovak Technical University, Bratislava, SK-812 37, Slovakia
SOURCE: Tetrahedron Letters (2000), 41(27), 5257-5260
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:238268
IT 293309-57-6P 293309-58-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of syn-γ-hydroxo-α-amino acids by stereoselective sodium borohydride reduction of γ-oxo-α-amino acids catalyzed by manganese(II) chloride)
RN 293309-57-6 HCAPLUS
CN 2-Thiophenebutanoic acid, γ-hydroxy-α-[(phenylmethyl)amino]-, (αR,γS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 293309-58-7 HCAPLUS
CN 2-Thiophenebutanoic acid, α-[(2-furanylmethyl)amino]-γ-hydroxy-5-methyl-, (αR,γS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L8 ANSWER 73 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

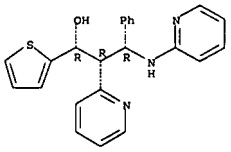
L8 ANSWER 74 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 14 Apr 2000
AB R1NHCHR2CHR3CHR4OH [I; R1 = (un)substituted 2-pyridyl; R2 = (un)substituted Ph; R3, R4 = (un)substituted Ph or heteroaryl] were prepared
Thus, 2-picoline was acylated by 5-methylthiophene-2-carboxylic acid and the product added to PhCH:NR1 (R1 = 2-pyridyl) (preparation given) to give,
after reduction, 4 diastereomers of I (R1 = R3 = 2-pyridyl, R2 = Ph, R4 = 5-methyl-2-thienyl). Data for biol. activity of I were given.
ACCESSION NUMBER: 2000:241215 HCAPLUS
DOCUMENT NUMBER: 132:265097
TITLE: Preparation of polyarylpropanolamines as hypolipemics
INVENTOR(S): Frick, Wendelin; Kirsch, Reinhard; Glombik, Heiner; Heuer, Hubert
PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000020410	A1	20000413	WO 1999-EP6932	19990918
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19845402	A1	20000413	DE 1998-19845402	19981002
DE 19845402	B4	20050407		
CA 2346083	A1	20000413	CA 1999-2346083	19990918
AU 9961925	A1	20000426	AU 1999-61925	19990918
AU 760412	B2	20030515		
EP 1117661	A1	20010725	EP 1999-948790	19990918
EP 1117661	B1	20040526		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9914266	A	20011106	BR 1999-14266	19990918
TR 200100895	T2	20011221	TR 2001-200100895	19990918
HU 200103893	A2	20020529	HU 2001-3893	19990918
JP 2002526539	T	20020820	JP 2000-574523	19990918
RU 2219176	C2	20031220	RU 2001-111815	19990918
AT 267825	T	20040615	AT 1999-948790	19990918
PT 1117661	T	20040930	PT 1999-948790	19990918
ES 2219065	T3	20041116	ES 1999-948790	19990918
US 6303639	B1	20011016	US 1999-407973	19990929
ZA 2001002589	A	20011219	ZA 2001-2589	20010329
HK 1040249	A1	20050401	HK 2002-102007	20020315
PRIORITY APPLN. INFO.:			DE 1998-19845402 A	19981002
			WO 1999-EP6932 W	19990918

OTHER SOURCE(S): MARPAT 132:265097
IT 263360-18-5P 263360-19-6P 263360-20-9P

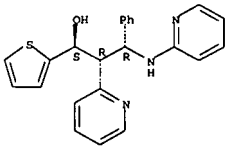
L8 ANSWER 74 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
263360-21-0P 263360-23-2P 263360-24-3P
263360-25-4P 263360-26-5P 263360-27-6P
263360-34-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of polyarylpropanolamines as hypolipemics)
RN 263360-18-5 HCAPLUS
CN 2-Pyridineethanol, β-[(R)-phenyl(2-pyridinylamino)methyl]-α-2-thienyl-, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 263360-19-6 HCAPLUS
CN 2-Pyridineethanol, β-[(R)-phenyl(2-pyridinylamino)methyl]-α-2-thienyl-, (αS,βR)-rel- (9CI) (CA INDEX NAME)

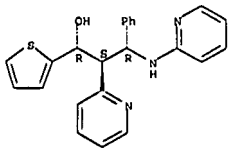
Relative stereochemistry.



RN 263360-20-9 HCAPLUS
CN 2-Pyridineethanol, β-[(R)-phenyl(2-pyridinylamino)methyl]-α-2-thienyl-, (αR,βS)-rel- (9CI) (CA INDEX NAME)

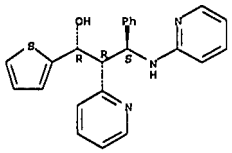
Relative stereochemistry.

L8 ANSWER 74 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

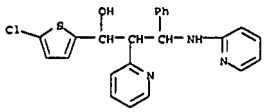


RN 263360-21-0 HCAPLUS
CN 2-Pyridineethanol, β-[(R)-phenyl(2-pyridinylamino)methyl]-α-2-thienyl-, (αS,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



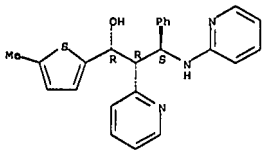
RN 263360-23-2 HCAPLUS
CN 2-Pyridineethanol, α-(5-chloro-2-thienyl)-β-[phenyl(2-pyridinylamino)methyl]- (9CI) (CA INDEX NAME)



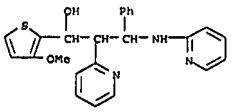
RN 263360-24-3 HCAPLUS
CN 2-Pyridineethanol, α-(5-methyl-2-thienyl)-β-[(R)-phenyl(2-pyridinylamino)methyl]-, (αR,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 74 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



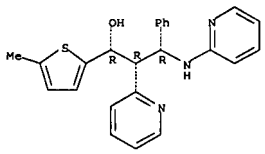
RN 263360-34-5 HCAPLUS
CN 2-Pyridineethanol, α-(3-methoxy-2-thienyl)-β-[phenyl(2-pyridinylamino)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

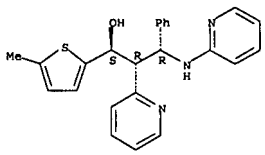
FORMAT

L8 ANSWER 74 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



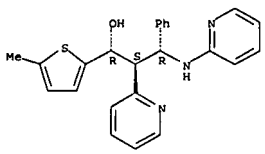
RN 263360-25-4 HCAPLUS
CN 2-Pyridineethanol, α-(5-methyl-2-thienyl)-β-[(R)-phenyl(2-pyridinylamino)methyl]-, (αS,βR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 263360-26-5 HCAPLUS
CN 2-Pyridineethanol, α-(5-methyl-2-thienyl)-β-[(R)-phenyl(2-pyridinylamino)methyl]-, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



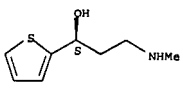
RN 263360-27-6 HCAPLUS
CN 2-Pyridineethanol, α-(5-methyl-2-thienyl)-β-[(R)-phenyl(2-pyridinylamino)methyl]-, (αS,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 75 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 18 Jan 2000
AB Sodium borohydride reduction of 3-chloro-1-(2-thienyl)-1-propanone gave the corresponding racemic alc., which was kinetically resolved with lipase B from Candida antarctica as catalyst to yield the chiral building blocks (S)-3-chloro-1-(2-thienyl)-1-propanol and the corresponding (R)-butanoate. The enantiopure chiral building blocks were converted to duloxetine and its enantiomer.

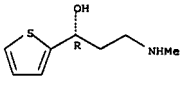
ACCESSION NUMBER: 2000:42097 HCAPLUS
DOCUMENT NUMBER: 132:207719
TITLE: Chemo-enzymatic synthesis of the antidepressant duloxetine and its enantiomer
AUTHOR(S): Liu, Huiling; Hoff, Bard Helge; Anthonsen, Thorleif
CORPORATE SOURCE: Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway
SOURCE: Chirality (2000), 12(1), 26-29
CODEN: CHRLEP; ISSN: 0899-0042
PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:207719
IT 116539-55-0P 116539-57-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(chemo-enzymic synthesis of duloxetine and its enantiomer)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

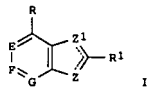


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

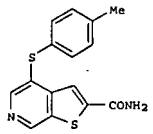
FORMAT

L8 ANSWER 75 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L8 ANSWER 76 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 10 Dec 1999
GI



I



II

AB Title compds. [I; EF:G = (un)substituted NCH:CH, -CHN:CH, -NCH:N, etc.; R = Z1R2; R1 = Z3R3; R2 = H, halo, alkyl, alkoxy, aryl, etc.; R3 = H, alkyl, alkoxy, aryl, CONH2, etc.; Z, Z1 = (un)substituted CH, -CH2, -NH, N, O, SO0-2; Z2,Z3 = bond, O, S, (alkyl)imino, CO, etc.; dashed lines = optional position of optional addnl. bond], inhibitors of e-selectin and ICAM-1 expression, were prepared Thus, 3,5-dichloropyridine was carbonylated and the product thioetherified by 4-MeC6H4SH to give 3-(4-methylphenylthio)-5-chloro-4-pyridinecarboxaldehyde which was cyclocondensed with HSCH2CO2Me to give, in 2 addnl. steps, title compound II. Data for biol. activity of I were given.

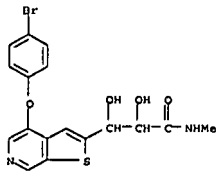
ACCESSION NUMBER: 1999:784103 HCAPLUS
DOCUMENT NUMBER: 132:22956
TITLE: Preparation of thienopyrimidinecarboxamides and analogs as cell adhesion-inhibiting antiinflammatory compounds
INVENTOR(S): Stewart, Andrew O.; Boyd, Steven A.; Arendsen, David L.; Bhatia, Pramila; Condroski, Kevin R.; Freeman, Jennifer C.; Gunawardana, Indrani W.; Zhu, Gui-Dong; Lartey, Kraig; McCarty, Catherine M.; Mort, Nicholas A.; Patel, Meena V.; Staeger, Michael A.; Stout, David M.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 282 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9962908	A2	19991209	WO 1999-US12419	19990603
WO 9962908	A3	20000330		

L8 ANSWER 76 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2333770	A1	19991209	CA 1999-2333770	19990603
AU 9942312	A	19991220	AU 1999-42312	19990603
EP 1090009	A2	20010411	EP 1999-926157	19990603
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
TR 200100189	T2	20010521	TR 2001-200100189	19990603
HU 200102366	A2	20011128	HU 2001-2366	19990603
BR 9910864	A	20020205	BR 1999-10864	19990603
JP 2002517396	T	20020618	JP 2000-552119	19990603
IN 2000MN00668	A	20050318	IN 2000-MN668	20001124
NO 2000006157	A	20010202	NO 2000-6157	20001204
BG 105109	A	20011130	BG 2001-105109	20010103
PRIORITY APPLN. INFO.:			US 1998-90701 A	19980604
			IN 1997-BO518 A3	19970904
			WO 1999-US12419 W	19990603

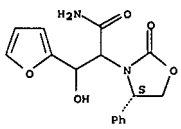
OTHER SOURCE(S): MARPAT 132:22956
IT 251995-08-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thienopyrimidinecarboxamides and analogs as cell adhesion-inhibiting antiinflammatory compds.)
RN 251995-08-1 HCAPLUS
CN Thieno[2,3-c]pyridine-2-propanamide, 4-(4-bromophenoxy)-α,β-dihydroxy-N-methyl- (9CI) (CA INDEX NAME)



L8 ANSWER 77 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 07 Sep 1998
AB A general approach to the solution phase parallel synthesis of perhydrooxazin-4-ones, which allows the preparation of milligram quantities of each individual member, is reported. An efficient purification method, using as "Sequestration Enabling Reagent" (SER) aminomethylpolystyrene resin in the presence of trimethylorthoformate is also described.

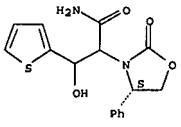
ACCESSION NUMBER: 1998:567490 HCAPLUS
DOCUMENT NUMBER: 129:260410
TITLE: Solution phase library of perhydrooxazin-4-ones
AUTHOR(S): Panunzio, Mauro; Villa, Marzia; Missio, Andrea; Rossi, Tino; Seneci, Pierfausto
CORPORATE SOURCE: CSFM-CNR Dipartimento di Chimica "G. Ciamician", Bologna, 40126, Italy
SOURCE: Tetrahedron Letters (1998), 39(36), 6585-6588
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 213335-83-2P 213335-85-4P 213335-93-4P
RL: BYP (Byproduct); PREP (Preparation)
(solution phase parallel synthesis of a perhydrooxazinone library)
RN 213335-83-2 HCAPLUS
CN 3-Oxazolidineacetamide, α-(2-furanylhydroxymethyl)-2-oxo-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



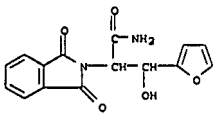
RN 213335-85-4 HCAPLUS
CN 3-Oxazolidineacetamide, α-(hydroxy-2-thienylmethyl)-2-oxo-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



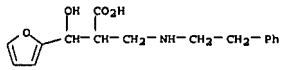
RN 213335-93-4 HCAPLUS

L8 ANSWER 77 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2H-Isoindole-2-acetamide, α-(2-furanylhydroxymethyl)-1,3-dihydro-1,3-dioxo- (9CI) (CA INDEX NAME)

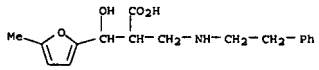


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 78 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 31 Jul 1998
AB An efficient method for the solid phase synthesis of allylic alcs. via the
Baylis-Hillman reaction has been developed. In the presence of DABCO or 3-quinuclidinol the coupling of resin bound acrylic acid with different aldehydes yields allylic alcs. Aldehydes with different reactivity were used and gave modest to excellent yields upon simply varying the base or the reaction time. The allylic alcs. were reacted with primary amines to form 1,3-aminoalcs.
ACCESSION NUMBER: 1998:474807 HCAPLUS
DOCUMENT NUMBER: 129:189195
TITLE: Solid phase synthesis of allylic alcohols via the Baylis-Hillman reaction
AUTHOR(S): Richter, Hartmut; Jung, Gunther
CORPORATE SOURCE: Institut fur Organische Chemie, Eberhard-Karls-Universitaet Tuebingen, Tuebingen, D-72076, Germany
SOURCE: Molecular Diversity (1998), Volume Date 1997-1998, 3(3), 191-194
CODEN: MODIF4; ISSN: 1381-1991
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:189195
IT 211917-12-3P 211917-14-5P 211917-17-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid phase synthesis of allylic alcs. via the Baylis-Hillman reaction)
RN 211917-12-3 HCAPLUS
CN 2-Furanpropanoic acid, β-hydroxy-α-[[(2-phenylethyl)amino]methyl]- (9CI) (CA INDEX NAME)

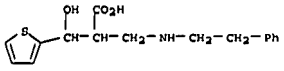


RN 211917-14-5 HCAPLUS
CN 2-Furanpropanoic acid, β-hydroxy-5-methyl-α-[[(2-phenylethyl)amino]methyl]- (9CI) (CA INDEX NAME)



RN 211917-17-8 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-[[(2-phenylethyl)amino]methyl]- (9CI) (CA INDEX NAME)

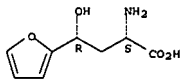
L8 ANSWER 78 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 79 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 19 Jun 1998
AB Kynureninase, which is known to catalyze the trans-aldol reaction between PhCHO and kynurenine, accepted many kinds of other aromatic aldehydes and propargyl aldehydes as substrates to afford novel γ-hydroxy α-L-amino acids. The L-configuration of the α-C atoms was confirmed by an enzymic method using both D- and L-amino acid oxidases. The absolute configuration of the newly formed chiral center (γ-position) in the major isomers is R, as determined by NMR of lactones derived from the γ-hydroxy α-L-amino acids.
ACCESSION NUMBER: 1998:376562 HCAPLUS
DOCUMENT NUMBER: 129:41390
TITLE: Kynureninase in organic synthesis. Preparation of γ-hydroxy α-L-amino acids
AUTHOR(S): Miura, Tsuyoshi; Masuo, Noriko; Fusamae, Yuki; Kajimoto, Tetsuya; Ida, Yoshiteru
CORPORATE SOURCE: School Pharmaceutical Sciences, Showa University, Tokyo, 142, Japan
SOURCE: Synlett (1998), (6), 631-633
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:41390
IT 208459-40-9P
RL: BPN (Biosynthetic preparation); PRP (Properties); RCT (Reactant); BIOL
(Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation by kynureninase-catalyzed asym. aldol reaction and absolute configuration)
RN 208459-40-9 HCAPLUS
CN 2-Furanbutanoic acid, α-amino-γ-hydroxy-, (αS,γR)- (9CI) (CA INDEX NAME)

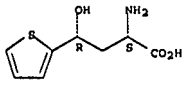
Absolute stereochemistry.



IT 208459-38-5P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of hydroxy amino acids by kynureninase-catalyzed asym. aldol reaction)
RN 208459-38-5 HCAPLUS
CN 2-Thiophenebutanoic acid, α-amino-γ-hydroxy-, (αS,γR)- (9CI) (CA INDEX NAME)

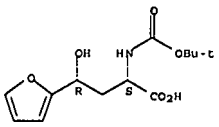
Absolute stereochemistry.

L8 ANSWER 79 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

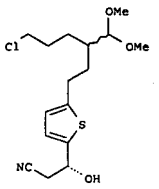


IT 208459-41-0P
RL: BPN (Biosynthetic preparation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hydroxy amino acids by kynureninase-catalyzed asym. aldol reaction)
RN 208459-41-0 HCAPLUS
CN 2-Furanbutanoic acid, α-[[(1,1-dimethylethoxy)carbonyl]amino]-γ-hydroxy-, (αS,γR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 80 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 18 Nov 1996
GI



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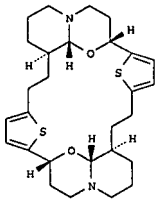


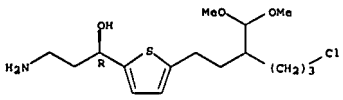
II

AB Xestospongin A, also known as araguspongine D, a C2-sym. macrocyclic alkaloid isolated from the sponge Xestospongia exigua (Xestospongia sp.), and its C(9) epimer xestospongin C, also known as araguspongine E, were synthesized. The route capitalized on the facile condensation between 5-halovaleraldehydes and 1,3-aminoalcs. to produce an oxaquinolizidine ring system in which all proper relative stereochem. relationships were controlled by equilibration. Thus, alc. I was converted to the key macrocyclic intermediate dimer II, which was subsequently hydrogenated in the presence of Raney Ni to form (+)-xestospongin A.

ACCESSION NUMBER: 1996:679156 HCAPLUS
DOCUMENT NUMBER: 126:47403
TITLE: Synthesis of the C2-Symmetric, Macrocyclic Alkaloid, (+)-Xestospongin A and Its C(9)-Epimer, (-)-Xestospongin C: Impact of Substrate Rigidity and Reaction Conditions on the Efficiency of the Macrocyclic Dimerization Reaction
AUTHOR(S): Hoye, Thomas R.; North, Jeffrey T.; Yao, Letitia J.; Ye, Zhixiong
CORPORATE SOURCE: Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Journal of the American Chemical Society (1996), 118(48), 12074-12081
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:47403
IT 184363-90-4P 184363-94-8P 184363-95-9P 184364-00-9P 184364-49-6P 184364-53-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of the macrocyclic alkaloid, (+)-xestospongin A, and its

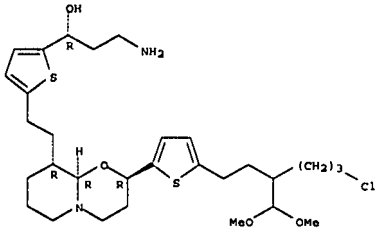
L8 ANSWER 80 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
C(9)-epimer, (-)-xestospongin C)
RN 184363-90-4 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-[6-chloro-3-(dimethoxymethyl)hexyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 184363-94-8 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-[2-[2-[5-[6-chloro-3-(dimethoxymethyl)hexyl]-2-thienyl]hexahydro-2H,6H-pyrido[2,1-b][1,3]oxazin-9-yl]ethyl]-, [2R-[2α,9β(R*),9aβ]]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



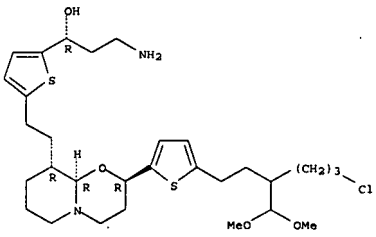
RN 184363-95-9 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-[2-[2-[5-[6-chloro-3-(dimethoxymethyl)hexyl]-2-thienyl]hexahydro-2H,6H-pyrido[2,1-b][1,3]oxazin-9-yl]ethyl]-, [2R-[2α,9β(R*),9aβ]]-[partial]-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 184363-94-8
CMF C30 H47 Cl N2 O4 S2

Absolute stereochemistry.

L8 ANSWER 80 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

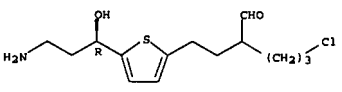
CRN 76-05-1
CMF C2 H F3 O2

RN 184364-00-9 HCAPLUS
CN 2-Thiophenebutanal, 5-(3-amino-1-hydroxypropyl)-α-(3-chloropropyl)-, (1R)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 184363-99-3
CMF C14 H22 Cl N O2 S

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

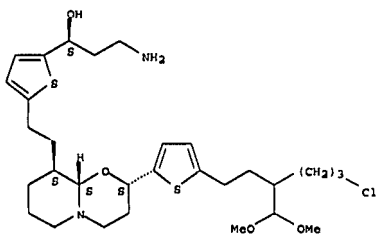
L8 ANSWER 80 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 184364-49-6 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-[2-[2-[5-[6-chloro-3-(dimethoxymethyl)hexyl]-2-thienyl]hexahydro-2H,6H-pyrido[2,1-b][1,3]oxazin-9-yl]ethyl]-, [2S-[2α,9β(R*),9aβ]]-[partial]-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 184364-48-5
CMF C30 H47 Cl N2 O4 S2

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

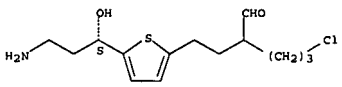
RN 184364-53-2 HCAPLUS
CN 2-Thiophenebutanal, 5-(3-amino-1-hydroxypropyl)-α-(3-chloropropyl)-, (1S)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

L8 ANSWER 80 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 184364-52-1
CMF C14 H22 Cl N O2 S

Absolute stereochemistry.

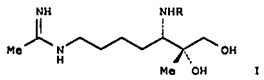


CM 2

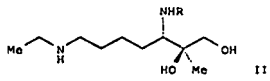
CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 81 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Dec 1995
GI



I



II

AB Novel amino glycol deriva. of L-N6-(1-iminoethyl)lysine represented by the general formula YC(:NR4)NR3XCH(NR1R2)-A-B [Y = H, each (un)substituted alkyl, alkenyl, alkynyl, aromatic hydrocarbyl, alicyclic hydrocarbyl, NH2, or heterocyclyl containing 1-4 heteroatoms selected from O, N, and S; X = alkyl, alkenyl, alkynyl, aromatic hydrocarbyl, (CH2)mQ(CH2)n (wherein m = 1-3, n = 1-3; Q = S, S(O), SO2, O, CO, etc.); R1 - R4 = H, alkyl; A = CO, each (un)substituted alkyl, alkenyl, alkynyl, alicyclic hydrocarbyl, or heterocyclyl containing 1-4 heteroatoms selected from O, N, and S; B = H, each (un)substituted alkyl, alkenyl, alkynyl, alkoxy, OH, alkoxycarbonyl, alkylaryloxy, thiol, alkylthio, alkylarylthio, arylthio, alkylsulfinyl, alkylarylsulfinyl, arylsulfinyl, alkylsulfonyl, alkylarylsulfonyl, arylsulfonyl, aromatic or alicyclic hydrocarbyl, or heterocyclyl containing 1-4 heteroatoms selected from O, N, and S; or B = CO2R5, CONR5R6, P(O)(OR5)OR6, NHOH, N(OH)CO NR5R6, NR5C(O)NR6R7, NR5CON(OH)R6, CONHOH; where R5, R6, R7 = H, each (un)substituted alkyl, aromatic or aliphatic hydrocarbyl] are prepared Thus, Z-Lys(Boc)-N(OMe)Me and Me2NCH2CH2NMe2 were dissolved in THF, treated a 1.4 M solution of MeLi in Et2O at -78°, and stirred at the same temperature for 3 h to give (S)-BocNH(CH2)4CH(NHZ)COMe, which was condensed with methyltriphenylphosphonium bromide in the presence of potassium hexamethyldisilazide in PhMe at -20° for 1.5 h to give (S)-BocNH(CH2)4CH(NHZ)C(:CH2)Me. The latter compound was hydroxylated by OsO4 and N-methylmorpholine in a mixture of acetone, H2O, and MeJCOH to give the diol BocNH(CH2)4CH(NHZ)CMe(OH)CH2OH which was deprotected with 4 N HCl in dioxane to HCl.H2N(CH2)4CH(NHZ)CMe(OH)CH2OH and condensed with Me acetimidate hydrochloride in DMF containing Et3N to give, after reversed phase column chromatog. using a YMC AQ-363-10P ODS column, the diastereoisomers (I and II; R = Z). The latter compds. were reduced under catalytic hydrogenation conditions using Pd-C at 5 psi H to give the title N-(iminoethyl)lysinol compds. I and II (R = H), which showed IC50 of 9.3 and 187 μM, resp., against human inducible nitric

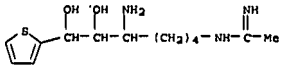
L8 ANSWER 81 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
oxide synthase.

ACCESSION NUMBER: 1995:994873 HCAPLUS
DOCUMENT NUMBER: 124:117978
TITLE: Preparation of L-N6-(1-iminoethyl)lysine derivatives useful as nitric oxide synthase inhibitors
INVENTOR(S): Hallinan, E. Ann; Tjoeng, Foe S.; Fok, Kam F.; Hagen, Timothy J.; Toth, Mihaly V.; Tsymbalov, Sofya; Pitzele, Barnett S.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: PCT Int. Appl., 106 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9524382	A1	19950914	WO 1995-US2669	19950308
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TT, UA				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2184691	A1	19950914	CA 1995-2184691	19950308
CA 2184691	C	20060221		
AU 9521156	A	19950925	AU 1995-21156	19950308
EP 749418	A1	19961227	EP 1995-913969	19950308
EP 749418	B1	20000830		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 195933	T	20000915	AT 1995-913969	19950308
ES 2151055	T3	20001216	ES 1995-913969	19950308
PT 749418	T	20010131	PT 1995-913969	19950308
US 6143790	A	20001107	US 1996-702695	19960906
GR 3034576	T3	20010131	GR 2000-402265	20001006
PRIORITY APPLN. INFO.:			US 1994-209094 A2	19940310
			WO 1995-US2669 W	19950308

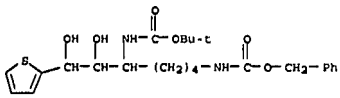
OTHER SOURCE(S): MARPAT 124:117978
IT 172832-94-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(iminoethyl)lysinol deriva. as nitric oxide synthase inhibitors)
RN 172832-94-9 HCAPLUS
CN Ethanimidamide, N-[5-amino-6,7-dihydroxy-7-(2-thienyl)heptyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 81 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

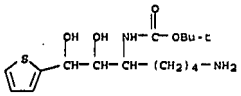


●2 HCl

IT 172833-72-6P 172833-73-7P 172833-74-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-(iminoethyl)lysinol derivs. as nitric oxide synthase inhibitors)
RN 172833-72-6 HCAPLUS
CN Carbamic acid, [1-[1,2-dihydroxy-2-(2-thienyl)ethyl]-5-[[(phenylmethoxy)carbonyl]amino]pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

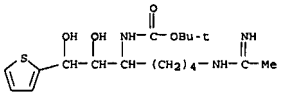


RN 172833-73-7 HCAPLUS
CN Carbamic acid, [5-amino-1-[1,2-dihydroxy-2-(2-thienyl)ethyl]pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 172833-74-8 HCAPLUS
CN Carbamic acid, [1-[1,2-dihydroxy-2-(2-thienyl)ethyl]-5-[(1-iminoethyl)amino]pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

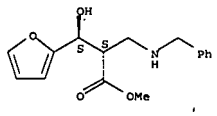
L8 ANSWER 81 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 82 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Sep 1995
AB A three-step process is presented for the preparation of α-substituted-β-amino esters which can serve as precursors to a key intermediate in carbapenem synthesis. The pivotal reaction in this sequence involves a highly diastereoselective conjugate addition reaction. Two series of alkenoates bearing a stereogenic substituent attached to C-2 were prepared and their conjugate addition reactions with benzylamine studied under several different sets of conditions. Conjugate addition of benzylamine to (R*)-RO2CC(:CH2)CHR1OSiMe2CMe3 [1, R = Me, CMe3, R1 = Me] in methanol at room temperature, gave the anti adducts PhCH2NHCH2CH(CO2R)CHR1OSiMe2CMe3 with virtually complete anti diastereoselectivity. These two β-amino esters bear the correct relative stereochem. and side chain to serve as precursors for carbapenem antibiotic synthetic intermediates. The role of the allylic substituents of I [R = Me, CMe3; R1 = Me, Et, CHMe2, Ph, 2-furyl] in determining the stereochem. outcome of these addns. is discussed.
These conjugate addns. were explored further by the preparation and conjugate addition reactions of the α,β-disubstituted alkenoates (E,Z)-R2CH:C(CO2Me)CHMeOSiMe2CMe3 [R2 = Me, CH2CH2OCH2Ph]. It was found that the presence of a β-substituent led to a dramatic reduction in yield although the same anti diastereoselectivity was maintained. The relative stereochem. of the adducts was established by examination of the relevant coupling consts. in the 1H NMR spectra of their tetrahydro-1,3-oxazine derivs.
ACCESSION NUMBER: 1995:806988 HCAPLUS
DOCUMENT NUMBER: 123:313598
TITLE: A Simple Route to α-Substituted-β-Amino Ester Precursors of Carbapenem Antibiotics
AUTHOR(S): Perlmutter, Patrick; Tabone, Mark
CORPORATE SOURCE: Department of Chemistry, Monash University, Clayton, 3168, Australia
SOURCE: Journal of Organic Chemistry (1995), 60(20), 6515-22
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:313598
IT 169900-39-4P 169900-40-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino ester carbapenem precursors via stereoselective conjugate addition reaction)
RN 169900-39-4 HCAPLUS
CN 2-Furanpropanoic acid, β-hydroxy-α-[[(phenylmethyl)amino]methyl]-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

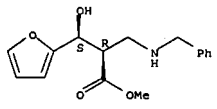
Relative stereochemistry.

L8 ANSWER 82 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 169900-40-7 HCAPLUS
CN 2-Furanpropanoic acid, β-hydroxy-α-[[(phenylmethyl)amino]methyl]-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

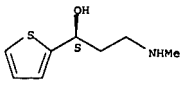
Relative stereochemistry.



L8 ANSWER 83 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 11 Mar 1995
AB Two 14C-isotopomers of duloxetine HCl [S-(+)-N-methyl-γ-(1-naphthalenyloxy)-2-thiophenepropanamine hydrochloride] have been prepared by an asym. synthesis. The palladium catalyzed cross-coupling of 2-thienoyl chloride (or its [carbonyl-14C] isotopomer) with vinyltributylstannane, followed by addition of HCl afforded the key pro-chiral intermediate chloro ketone. Chiral reduction with borane in the presence of the appropriate oxazaborolidine catalyst provided the S-chloro alc. and its 14C-labeled counterpart or the analogous R-chloro alc. Activation of the chloro alcs. by reaction with NaI/acetone, followed by reaction of the corresponding iodo alcs. with methylamine yielded the penultimate amino alcs. Formation of the alkoxide with NaH, followed by reaction with 1-fluoronaphthalene yielded duloxetine or its 14C-labeled isotopomer. Alternatively, reaction of the R-chloro alc. with 1-naphthol-[1-14C] under Mitsunobu conditions afforded a aryl ether, which was in turn activated by reaction with NaI/acetone. Subsequent reaction with methylamine followed by salt formation yielded duloxetine or its naphthalene-labeled isotopomer as their HCl salts.
ACCESSION NUMBER: 1995:409881 HCAPLUS
DOCUMENT NUMBER: 123:55626
TITLE: An asymmetric synthesis of duloxetine hydrochloride, a mixed uptake inhibitor of serotonin and norepinephrine, and its C-14 labeled isotopomers
AUTHOR(S): Wheeler, William J.; Kuo, Fengjiun
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly Co., Indianapolis, IN, 46285, USA
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1995), 36(3), 213-23
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:55626
IT 116539-55-0P 164071-60-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of duloxetine hydrochloride and its carbon-14 labeled isotopomers)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

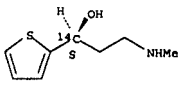
Absolute stereochemistry. Rotation (+).

L8 ANSWER 83 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

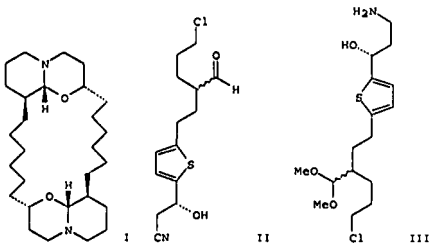


RN 164071-60-7 HCAPLUS
CN 2-Thiophenemethanol-α-14C, α-[2-(methylamino)ethyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



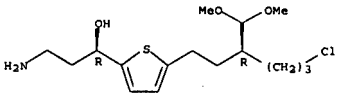
L8 ANSWER 84 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Jul 1994
GI



AB The title compound (I) was prepared in a multistep sequence starting from 5-chlorovaleronitrile and oxirane via coupling of the two halves II and III.
ACCESSION NUMBER: 1994:435943 HCAPLUS
DOCUMENT NUMBER: 121:35943
TITLE: A Total Synthesis of (+)-Xestospongin A/(+)-Araguspongine D
AUTHOR(S): Hoye, Thomas R.; North, Jeffrey T.; Yao, Letitia J.
CORPORATE SOURCE: Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Journal of the American Chemical Society (1994), 116(6), 2617-18
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:35943
IT 155988-59-3P 155988-62-8P 155988-64-0P 155988-68-4P 156041-29-1P 156041-31-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in total synthesis of xestospongin A)
RN 155988-59-3 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-[6-chloro-3-(dimethoxymethyl)hexyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

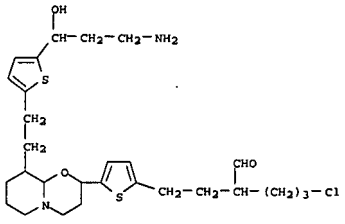
L8 ANSWER 84 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 155988-62-8 HCAPLUS
CN 2-Thiophenebutanal, 5-[9-[2-[5-(3-amino-1-hydroxypropyl)-2-thienyl]ethyl]hexahydro-2H,6H-pyrido[2,1-b][1,3]oxazin-2-yl]-α-(3-chloropropyl)-, [2R-[2α(R*),9β(R*),9aβ]]-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 155988-61-7
CMF C28 H41 Cl N2 O3 S2



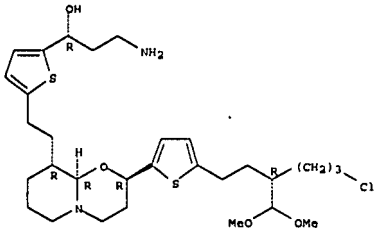
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 155988-64-0 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-[2-[2-[5-[6-chloro-3-(dimethoxymethyl)hexyl]-2-thienyl]hexahydro-2H,6H-pyrido[2,1-b][1,3]oxazin-9-yl]ethyl]-, [2R-[2α(R*),9β(R*),9aβ]]- (9CI) (CA INDEX NAME)

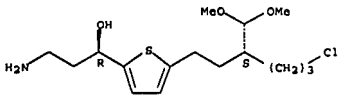
L8 ANSWER 84 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.



RN 155988-68-4 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-[6-chloro-3-(dimethoxymethyl)hexyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

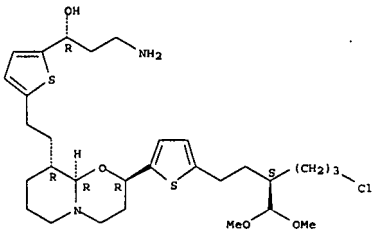


RN 156041-29-1 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)-5-[2-[2-[5-[6-chloro-3-(dimethoxymethyl)hexyl]-2-thienyl]hexahydro-2H,6H-pyrido[2,1-b][1,3]oxazin-9-yl]ethyl]-, [2R-[2α(S*),9β(R*),9aβ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 84 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

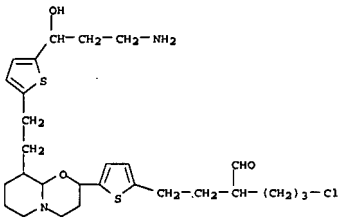
L8 ANSWER 84 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 156041-31-5 HCAPLUS
CN 2-Thiophenebutanal, 5-[9-[2-[5-(3-amino-1-hydroxypropyl)-2-thienyl]ethyl]hexahydro-2H,6H-pyrido[2,1-b][1,3]oxazin-2-yl]-α-(3-chloropropyl)-, [2R-[2α(S*),9β(R*),9aβ]]-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

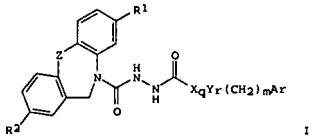
CRN 156041-30-4
CMF C28 H41 Cl N2 O3 S2



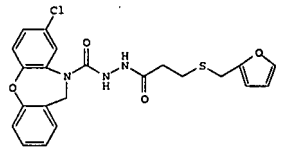
CM 2

CRN 76-05-1
CMF C2 H F3 O2

L8 ANSWER 85 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 19 Mar 1993
GI



I



II

AB Title compds. [I; R1 = H, halo, CF3; R2 = H, halo, OH, OMe; Z = O, S, SO, SO2; X = CH:CH, CF2, CHF, (CH2)n, (CH2)pCH:CH; Y = CH(OH), NR3, S, SO, SO2, O; q, r = 0, 1; m = 0-6; n, p = 1-6; R3 = H, Me3CO2C; Ar = (substituted) aryl] were prepared Thus, 3-[(2-furylmethyl)thio]propanoic acid hydrazide (prepn given) and 8-chlorodibenz[b,f][1,4]oxazepine-10(11H)-carbonyl chloride (preparation given) were condensed in PhMe containing Et3N at reflux to give 100% title compound II. II showed ED50 = 0.9 mg/kg in the phenylbenzoquinone-induced writhing test in mice, and antagonized prostaglandin E2 in guinea pig ileum with pA2 = 8.5.

ACCESSION NUMBER: 1993:102002 HCAPLUS
DOCUMENT NUMBER: 118:102002
TITLE: Preparation of dibenz[b,f][1,4]oxazepines and related compounds as analgesics and prostaglandin antagonists
INVENTOR(S): Hallinan, E. Ann; Hagen, Timothy Joseph; Husa, Robert Knol; Teymbalov, Sofya; Lee, Albert C.; Van Hoeck, Jean Pierre
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: Eur. Pat. Appl., 61 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 512400	A1	19921111	EP 1992-107328	19920429
EP 512400	B1	19981202		

L8 ANSWER 85 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

R: PT					
CA 2108903	A1	19921104	CA 1992-2108903		19920416
CA 2108903	C	20040210			
WO 9219617	A2	19921112	WO 1992-US3028		19920416
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US					
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG					
AU 9222462	A	19921221	AU 1992-22462		19920416
EP 583421	A1	19940223	EP 1992-914560		19920416
EP 583421	B1	19990616			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE					
JP 06507408	T	19940825	JP 1992-511838		19920416
JP 3222891	B2	20011029			
EP 694545	A2	19960131	EP 1995-116871		19920416
EP 694545	A3	19960327			
EP 694545	B1	20000726			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE					
AT 181329	T	19990715	AT 1992-914560		19920416
ES 2133324	T3	19990916	ES 1992-914560		19920416
AT 194987	T	20000815	AT 1995-116871		19920416
ES 2149305	T3	20001101	ES 1995-116871		19920416
EP 694546	A2	19960131	EP 1995-116872		19920429
EP 694546	A3	19960327			
EP 694546	B1	20010606			
R: PT					
EP 911331	A2	19990428	EP 1999-101029		19920429
EP 911331	A3	20000119			
EP 911331	B1	20031022			
R: PT					
PT 694546	T	20010928	PT 1995-116872		19920429
PT 911331	T	20040331	PT 1999-101029		19920429
US 5378840	A	19950103	US 1993-108551		19930824
US 5464830	A	19951107	US 1994-295302		19940824
US 5576315	A	19961119	US 1995-509846		19950801
GR 3034650	T3	20010131	GR 2000-402337		20001020
PRIORITY APPLN. INFO.:			US 1991-695654	A	19910503
			WO 1992-US3028	A	19920416
			EP 1992-914560	A3	19920416
			EP 1992-107328	A3	19920429
			EP 1995-116872	A3	19920429
			US 1993-108551	A1	19930824
			US 1994-295302	A3	19940824

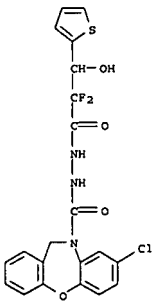
OTHER SOURCE(S): CASREACT 118:102002; MARPAT 118:102002

IT 146032-86-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as analgesic and prostaglandin antagonist)

RN 146032-86-2 HCAPLUS

L8 ANSWER 85 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

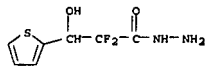
CN Dibenz[b,f][1,4]oxazepine-10(11H)-carboxylic acid, 8-chloro-, 2-[2,2-difluoro-3-hydroxy-1-oxo-3-(2-thienyl)propyl]hydrazide (9CI) (CA INDEX NAME)



IT 146033-30-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, intermediate for analgesics and prostaglandin antagonists)

RN 146033-30-9 HCAPLUS

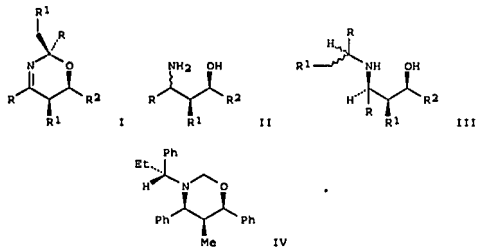
CN 2-Thiophenepropanoic acid, α,α-difluoro-β-hydroxy-, hydrazide (9CI) (CA INDEX NAME)



L8 ANSWER 86 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 23 Aug 1991

GI



AB 5,6-Dihydro-2H-1,3-oxazines I (R = Ph, R1 = Me, R2 = Ph, 2-thienyl, PhMeCH; R = R2 = Ph, R1 = Et; R = 4-MeC6H4, R1 = Me, R2 = 4-MeC6H4, Bu, Ph), prepared from cyclocondensation of R1CH:CRN:CRCH2R1 with R2CHO, react with Na/Me2CHOH to give the tetrahydro-2H-1,3-oxazines which undergo acid hydrolysis to give 1,3-amino alcs. II with three stereocenters. Reduction of I (R = Ph, R1 = Me, R2 = Ph, 2-thienyl, PhMeCH; R = R2 = Ph, R1 = Et) with LiAlH4 gives 1,3-amino alcs. III with four stereocenters. The stereochem. of these compds. was established by x-ray crystallog. of methyldiphenyl(phenylpropyl)oxazine IV.

ACCESSION NUMBER: 1991:471508 HCAPLUS

DOCUMENT NUMBER: 115:71508

TITLE: Synthesis of 1,3-amino alcohols from 2-aza-1,3-dienes by reduction of 5,6-dihydro-2H-1,3-oxazines

AUTHOR(S): Barluenga, Jose; Joglar, Jesus; Gonzalez, Francisco J.; Fustero, Santos; Krueger, Carl; Tsay, Y. H.

CORPORATE SOURCE: Fac. Quim., Univ. Oviedo, Oviedo, E-33071, Spain

SOURCE: Synthesis (1991), (5), 387-92
CODEN: SYNTBF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English

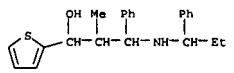
OTHER SOURCE(S): CASREACT 115:71508

IT 124315-32-8P 124338-11-0P 124378-68-3P 135092-77-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 124315-32-8 HCAPLUS

CN 2-Thiophenemethanol, α-[1-methyl-2-phenyl-2-[(1-phenylpropyl)amino]ethyl]-, [1R*(S*),2R*(R*)]- (9CI) (CA INDEX NAME)

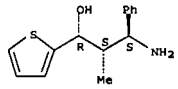
L8 ANSWER 86 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 124338-11-0 HCAPLUS

CN 2-Thiophenemethanol, α-(2-amino-1-methyl-2-phenylethyl)-, [1R*(S*),2R*]- (9CI) (CA INDEX NAME)

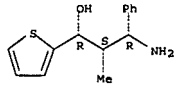
Relative stereochemistry.



RN 124378-68-3 HCAPLUS

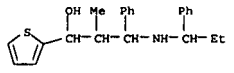
CN 2-Thiophenemethanol, α-(2-amino-1-methyl-2-phenylethyl)-, [1R*(S*),2S*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 135092-77-2 HCAPLUS

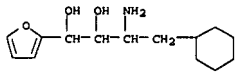
CN 2-Thiophenemethanol, α-[1-methyl-2-phenyl-2-[(1-phenylpropyl)amino]ethyl]-, [1R*(S*),2R*(S*)]- (9CI) (CA INDEX NAME)



L8 ANSWER 87 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 03 Aug 1990
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; R1 = H, Me; R2 = Et, Pr, heterocyclyl, MeJCO; R3 = Me2CHCH2, cyclohexylmethyl, Ph, CH2O; R4, R5 = H, (substituted) alkanoyl, (cyclic) protecting group; R6 = aralkyl, arylalkenyl; A = substituted alkanoyl, etc.], useful as antihypertensives, were prepared Aminohexanediol II (R = H) (preparation given) was condensed with FMOC-His-OH (FMOC = fluoranylmethoxycarbonyl) followed by deprotection to give II (R = Q), which was condensed with HO2CCH(CH2Ph)CH2COCMe3 to give I [R1 = R4 = R5 = H, R2 = 1H-imidazol-4-yl, R3 = cyclohexylmethyl, A = COCH(CH2Ph)CH2COCMe3]. This showed an IC50 of 0.024 μM against renin in vitro.
ACCESSION NUMBER: 1990:441323 HCAPLUS
DOCUMENT NUMBER: 113:41323
TITLE: Preparation of peptide-like amino acid derivatives as antihypertensives and pharmaceutical compositions containing them
INVENTOR(S): Branca, Quirico; Neidhart, Werner; Ramuz, Henri; Stadler, Heinz; Wostl, Wolfgang
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.
SOURCE: Eur. Pat. Appl., 49 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

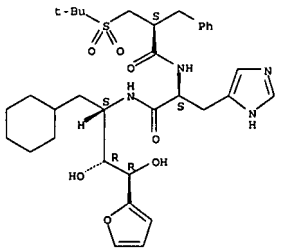
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 332008	A2	19890913	EP 1989-103416		19890227
EP 332008	A3	19920408			
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
CA 1328333	C	19940405	CA 1989-591212		19890216
ZA 8901464	A	19891227	ZA 1989-1464		19890224
DK 8900968	A	19890905	DK 1989-968		19890228
AU 8930797	A	19890907	AU 1989-30797		19890228
AU 617429	B2	19911128			
HU 50104	A2	19891228	HU 1989-992		19890301
FI 8901006	A	19890905	FI 1989-1006		19890302
JP 02003646	A	19900109	JP 1989-48693		19890302
JP 08009585	B	19960131			
NO 8900921	A	19890905	NO 1989-921		19890303
US 5134123	A	19920728	US 1989-318576		19890303
US 5256645	A	19931026	US 1992-872736		19920422
US 5389616	A	19950214	US 1993-99028		19930729
PRIORITY APPLN. INFO.:			CH 1988-820	A	19880304
			CH 1988-3469	A	19880916
			CH 1988-4824	A	19881228
			US 1989-318576	A3	19890303
			US 1992-872736	A3	19920422

L8 ANSWER 87 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 113:41323
IT 126223-07-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antihypertensive amino acid amides)
RN 126223-07-2 HCAPLUS
CN 1,2-Butanediol, 3-amino-4-cyclohexyl-1-(2-furanyl)- (9CI) (CA INDEX NAME)



IT 126222-59-1P 126371-85-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antihypertensive)
RN 126222-59-1 HCAPLUS
CN 1H-Imidazole-4-propanamide, N-[1-(cyclohexylmethyl)-3-(2-furanyl)-2,3-dihydroxypropyl]-α-[[2-[[(1,1-dimethylethyl)sulfonyl]methyl]-1-oxo-3-phenylpropyl]amino]-, [1S-[1R*[R*(R*)],2S*,3S*]]- (9CI) (CA INDEX NAME)

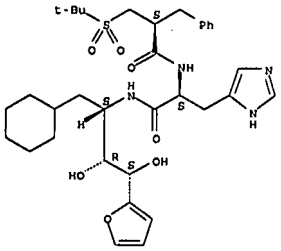
Absolute stereochemistry.



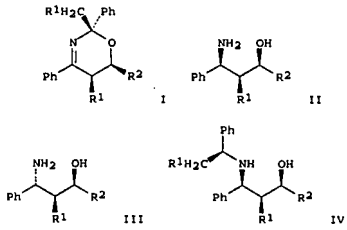
RN 126371-85-5 HCAPLUS
CN 1H-Imidazole-4-propanamide, N-[1-(cyclohexylmethyl)-3-(2-furanyl)-2,3-dihydroxypropyl]-α-[[2-[[(1,1-dimethylethyl)sulfonyl]methyl]-1-oxo-3-phenylpropyl]amino]-, [1S-[1R*[R*(R*)],2S*,3R*]]- (9CI) (CA INDEX NAME)

L8 ANSWER 87 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

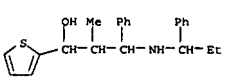
Absolute stereochemistry.



L8 ANSWER 88 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 21 Jan 1990
GI

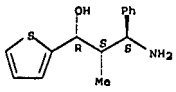


AB Dihydroxazines I (R1 = Me, Et; R2 = Ph, thienyl, PhCHMe) were reduced by Na-Me2CHOH to give mixts. of amino alc. isomers II and III. The treatment of I with LiAlH4 gave N-substituted amino alcs. IV and another epimer.
ACCESSION NUMBER: 1990:20949 HCAPLUS
DOCUMENT NUMBER: 112:20949
TITLE: Reduction of 5,6-dihydro-2H-1,3-oxazines. A simple approach to 1,3-aminoalcohols from 2-aza-1,3-dienes
AUTHOR(S): Barluenga, Jose; Joglar, Jesus; Gonzalez, Francisco J.; Fustero, Santos
CORPORATE SOURCE: Fac. Quim., Univ. Oviedo, Oviedo, 33071, Spain
SOURCE: Tetrahedron Letters (1989), 30(15), 2001-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:20949
IT 124315-32-8P 124338-11-0P 124377-44-2P 124378-68-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 124315-32-8 HCAPLUS
CN 2-Thiophenemethanol, α-[1-methyl-2-phenyl-2-[(1-phenylpropyl)amino]ethyl]-, [1R*(S*),2R*(R*)]- (9CI) (CA INDEX NAME)

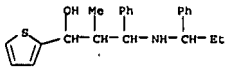


RN 124338-11-0 HCAPLUS
CN 2-Thiophenemethanol, α-(2-amino-1-methyl-2-phenylethyl)-, [1R*(S*),2R*]- (9CI) (CA INDEX NAME)

L8 ANSWER 88 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Relative stereochemistry.

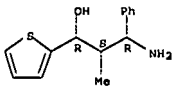


RN 124377-44-2 HCAPLUS
CN 2-Thiophenemethanol, α-[1-methyl-2-phenyl-3-[(1-phenylpropyl)amino]ethyl]-, [1R*(S*),2R*(S*)]- (9CI) (CA INDEX NAME)

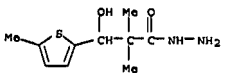


RN 124378-68-3 HCAPLUS
CN 2-Thiophenemethanol, α-(2-amino-1-methyl-2-phenylethyl)-, [1R*(S*),2S*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

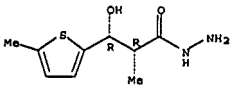


L8 ANSWER 89 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 117970-73-7 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α,α,5-trimethyl-, hydrazide (9CI) (CA INDEX NAME)

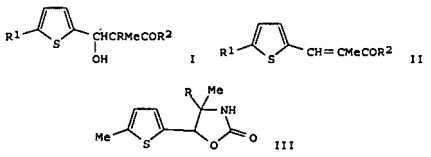


RN 117982-40-8 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α,5-dimethyl-, hydrazide, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

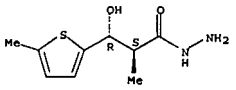


L8 ANSWER 89 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 06 Jan 1989
GI

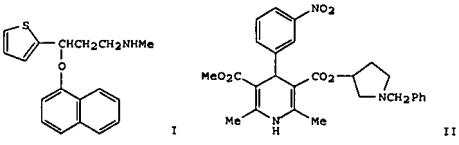


AB Reformatskii reaction of 5-methyl- or 5-bromo-2-thiophenecarboxaldehyde with BrCRMeCO2Et (R = H, Me) in C6H6 gave esters I [R = H, Me, R1 = Me; R2 = OEt (threo and erythro diastereomers)] and II (R1 = Me, Br; R2 = OEt), which reacted with N2H4.H2O to give the corresponding hydrazides in 39.99-93% yield. Curtius reaction of I (same R, R1; R2 = NHNH2) gave 61.65-79.49% thienyloxazolidinones III. I and II (R2 = NHNH2) and III were central nervous depressants with LD50 ≤1500 mg/kg.
ACCESSION NUMBER: 1989:7984 HCAPLUS
DOCUMENT NUMBER: 110:7984
TITLE: Substituted 3-(2-thienyl) carboxylic acids with central depressive activity
AUTHOR(S): Mavrova-Popivanova, A.; Zhelyazkov, L.
CORPORATE SOURCE: Bulg.
SOURCE: Farmatsiya (Sofia, Bulgaria) (1988), 38(1), 1-5
CODEN: FMTYA2; ISSN: 0428-0296
DOCUMENT TYPE: Journal
LANGUAGE: Bulgarian
OTHER SOURCE(S): CASREACT 110:7984
IT 117970-72-6P 117970-73-7P 117982-40-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, nervous system-depressant activity, and Curtius rearrangement of)
RN 117970-72-6 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α,5-dimethyl-, hydrazide, (R*,S*)- (9CI) (CA INDEX NAME)

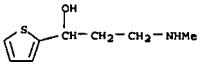
Relative stereochemistry.



L8 ANSWER 90 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 14 Oct 1988
GI



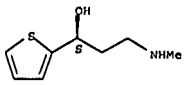
AB HPLC methods were developed to sep. some CNS drugs, both indirectly after diastereomer formation, and directly using chiral stationary phases. Some examples are: resolution of fluoxetine as mandelic acid derivative on a H2 column; resolution and determination of I as Mosher's acid derivative on a NH2 column or the acetylate I derivative on a Cyclobond I column; chromatog. of tomoxetine spiked with its (+)-isomer on a Cyclobond I column after acetylation; and chiral separation of the Ca channel blocker II on an α1-acid glycoprotein column.
ACCESSION NUMBER: 1988:535063 HCAPLUS
DOCUMENT NUMBER: 109:135063
TITLE: Practical considerations for chiral separations of pharmaceutical compounds
AUTHOR(S): Bopp, Ronald J.; Kennedy, Joseph H.
CORPORATE SOURCE: Lilly Corp. Cent., Eli Lilly Co., Indianapolis, IN, 46285, USA
SOURCE: LC-GC (1988), 6(6), 514, 516, 518, 520, 522
CODEN: LCGCE7; ISSN: 0888-9090
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 116539-56-1
RL: PROC (Process)
(resolution of, HPLC chiral phases for)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



IT 116539-55-0 116539-57-2
RL: PROC (Process)
(separation of, on HPLC chiral phases)
RN 116539-55-0 HCAPLUS

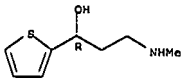
L8 ANSWER 90 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

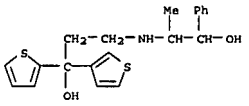


RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

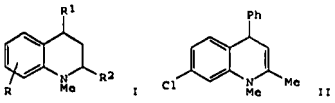


L8 ANSWER 91 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB The title compds. RR1XCH2NHCHMeCHPhOH·HCl I [R and R1 = Ph or thienyl; X = C(OH)CH2, C:CH or CHCH2] prepared by known methods were evaluated for their effect on cerebral blood flow in dogs. D 8974 (I; R = R1 = 3-thienyl, X = CHCH2 produced the highest increase in cerebral blood flow.
ACCESSION NUMBER: 1980:597538 HCAPLUS
DOCUMENT NUMBER: 93:197538
TITLE: New cerebrally active basic dithienyl compounds
AUTHOR(S): Thiele, K.; Poesselt, K.; Offermanns, H.; Thiemer, K.
CORPORATE SOURCE: Chemiewerk Homburg, Degussa, Frankfurt/Main, Fed. Rep. Ger.
SOURCE: Arzneimittel-Forschung (1980), 30(5), 747-51
CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE: Journal
LANGUAGE: German
IT 37750-25-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and brain circulation response to)
RN 37750-25-7 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-α-3-thienyl-, hydrochloride (9CI) (CA INDEX NAME)

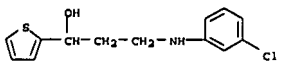


● HCl

L8 ANSWER 92 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI

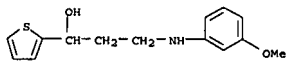


AB RC6H4NMeCHR2CH2CH(OH)R1 (R = 3-Cl, 3-MeO, R1 = 2-thienyl, R2 = H; R = 4-MeO, R1 = Ph, R2 = H; R = 3-Cl, R1 = Ph, R2 = Me) on cyclodehydration gave the corresponding N-methyl-1,2,3,4-tetrahydroquinolines I, which were converted to the methiodides. 7-Chloro-2-methyl-4-phenylquinoline was converted to the methiodide, which on NaBH4 reduction gave the 1,4-dihydroquinoline II. II was converted to the methiodide.
ACCESSION NUMBER: 1978:120954 HCAPLUS
DOCUMENT NUMBER: 88:120954
TITLE: Synthesis of heterocyclic compounds: part XXI. Dihydro- and tetrahydroquinolines and their methiodides
AUTHOR(S): Gogte, V. N.; Mukhedkar, V. A.; Tilak, B. D.
CORPORATE SOURCE: Natl. Chem. Lab., Poona, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1977), 15B(9), 774-7
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:120954
IT 55439-07-1P 65602-24-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 55439-07-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(3-chlorophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

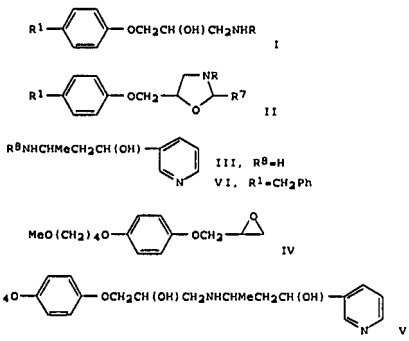


RN 65602-24-6 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(3-methoxyphenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 92 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 93 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI



AB The title compds. I [R = CR2:CHCOR3, CHR2CH2CH(OH)R3 (R2 = H, Me; R3 = an aromatic or quasi-aromatic 5- or 6-membered monocyclic ring, with 1 or 2 N, O, and (or) S atoms, which can be substituted with 1 or more Me groups, and connected via a C atom); R1 = alkoxymethyl, alkoxyalkoxy, hydroxyalkoxy, NHCONR4R5 (R4 and R5 = H, alkyl, alkenyl, cycloalkyl; NR4R5 = a saturated 5- or 6-membered heterocyclic group, which may have O or S as an addnl. heteroatom), and contain C1-4 alkyl or alkoxy groups, C3-4 alkenyl groups, or C5-7 cycloalkyl groups] as well as their aldehyde condensation products and acid addition salts, were prepared by treating 4-R1C6H4OCH2R6 [R6 = 2-oxiranyl, CH(OH)CH2X (X = halo) with H2NR (R as above) and the compds. formed, if necessary, converted with R7CHO (R7 = H, C1-4 alkyl) into the oxazolidine II, or, with acid into the acid addition salts. Thus, e.g., aminobutanol III in PhMe was treated with epoxide IV and the mixture stirred 36 h at room temperature to give the dihydroxyamine V. III was prepared by treating nicotinoylacetone K salt in EtOH with PhCH2NH2.HCl, stirring the mixture 24 h at room temperature (88% yield), reducing the product R9CH:CMeNHCH2Ph (R9 = nicotinoyl) with NaBH4 (62% yield), and debenzylating the amino alc.

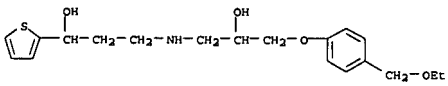
VI. An addnl. 57 I and 1 oxazolidine deriv. were prepd. Selected I had ED50 0.003-0.093 mg/kg (dog) as β1-receptor inhibitors and ED50 1.02-15.59 mg/kg (dog) as β2-receptor inhibitors [vs. 0.238 and 26.505 for 4-Me2CHNHCH2CH(OH)CH2OC6H4NHAc] and are useful in treating arrhythmia and other heart disorders.

ACCESSION NUMBER: 1978:105153 HCAPLUS
DOCUMENT NUMBER: 88:105153
TITLE: 1-Phenoxy-3-aminopropan-2-ol derivatives and their acid addition salts
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Austrian, 17 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

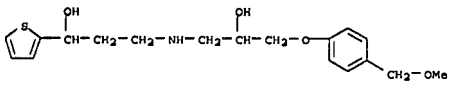
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 339307	B	19771010	AT 1974-10167	19741219
AT 7410167	A	19770215		
US 4088764	A	19780509	US 1974-531344	19741210
FI 7403631	A	19750628	FI 1974-3631	19741216
NO 7404530	A	19750630	NO 1974-4530	19741216
SE 7415761	A	19750630	SE 1974-15761	19741216
DK 7406547	A	19750825	DK 1974-6547	19741216
DD 117071	A5	19751220	DD 1974-183198	19741219
ZA 7408082	A	19760128	ZA 1974-8082	19741219
SU 559643	A3	19770525	SU 1974-2085461	19741219
SU 598557	A3	19780315	SU 1974-2085234	19741219
HU 171726	B	19780328	HU 1974-CA376	19741219
CA 1047512	A1	19790130	CA 1974-216421	19741219
US 4066768	A	19780103	US 1976-669995	19760324

PRIORITY APPLN. INFO.: LU 1973-34590 A 19731227
US 1974-531344 A2 19741210

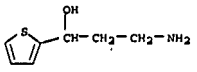
IT 57725-58-3P 65653-26-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57725-58-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[[3-[4-(ethoxymethyl)phenoxy]-2-hydroxypropyl]amino]ethyl]- (9CI) (CA INDEX NAME)



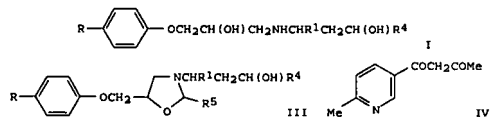
L8 ANSWER 93 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 65653-26-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[[2-hydroxy-3-[4-(methoxymethyl)phenoxy]propyl]amino]ethyl]- (9CI) (CA INDEX NAME)



IT 65653-31-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with glycidyl Ph ethers)
RN 65653-31-8 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 94 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI



AB A process was claimed for the preparation of the title compds. I [R = alkoxymethyl, alkoxyalkoxy, hydroxyalkoxy, NHCONR2R3 (R2 and R3 = H, alkyl, alkenyl, cycloalkyl; NR2R3 = a saturated 5- or 6-membered monocyclic heterocyclic group, if necessary, having an O or S as addnl. hetero atom, and containing C1-4 alkyl or alkoxy, C3-4 alkenyl, C5-7 cycloalkyl groups); R1 = H, Me; R4 = a C-bound aromatic or quasi-aromatic 5- or 6-membered monocyclic ring with 1 or 2 N, O, and(or) S atoms, which can be substituted by 1 or more Me groups] as well as their aldehyde condensation products and acid addition salts, whereby one hydrogenates 4-RC6H4OCH2CH(OH)CH2NHCR1:CHCOR4 (II), 4-RC6H4OCH2COCH2NHCR1:CHCOR4, or 4-RC6H4OCH2COCH2NHCHR1CH2CH(OH)R4, or, if one preps. I (R1 = H), one hydrogenates 4-RC6H4OCH2COCH2NHCH2CH2COR4 or 4-RC6H4OCH2CH(OH)CH2NHCH2CH2COR4 and one converts the compound formed into an oxazolidine III (R5 = H, C1-4 alkyl) with R5CHO, or, if necessary, with an acid into an acid addition salt. Thus, 4-MeO(CH2)4OC6H4OCH2CH(OH)CH2NH2, nicotinoylacetone IV, EtOH, and HCO2H were heated to 50° and stirred an addnl. 20 h at room temperature to give II [R = MeO(CH2)4O, R1 = Me, R4 = 2-methyl-5-pyridyl] which was reduced with NaBH4 at 70° in EtOH 7 h to give the corresponding I. IV was prepared by stirring 5-acetyl-α-picoline, PhMe, EtOAc, and KOCMe3 20 h at 40°. An addnl. 27 I, 2 I salts, and 1 III were prepared. Selected I had ED50 0.003-0.093 mg/kg (dog), as β1-receptor inhibitors and ED50 1.02-15.59 mg/kg (dog) as β2-receptor inhibitors [vs. 0.238 and 26.505 for 4-Me2CHNHCH2CH(OH)CH2OC6H4NHAc] and are useful in treating arrhythmia and other heart disorders.

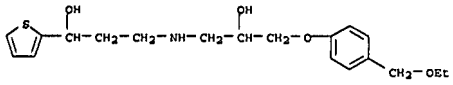
ACCESSION NUMBER: 1978:105151 HCAPLUS
DOCUMENT NUMBER: 88:105151
TITLE: 1-Phenoxy-3-aminopropan-2-ol derivatives and their acid addition salts
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Austrian, 14 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 339305	B	19771010	AT 1974-10164	19741219
AT 7410164	A	19770215		

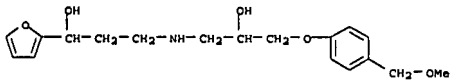
L8 ANSWER 94 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

US 4088764	A	19780509	US 1974-531344		19741210
FI 7403631	A	19750628	FI 1974-3631		19741216
NO 7404530	A	19750630	NO 1974-4530		19741216
SE 7415761	A	19750630	SE 1974-15761		19741216
DK 7406547	A	19750825	DK 1974-6547		19741216
DD 117071	A5	19751220	DD 1974-183198		19741219
ZA 7408082	A	19760128	ZA 1974-8082		19741219
SU 559643	A3	19770525	SU 1974-2085461		19741219
SU 598557	A3	19780315	SU 1974-2085234		19741219
HU 171726	B	19780328	HU 1974-CA376		19741219
CA 1047512	A1	19790130	CA 1974-216421		19741219
US 4066768	A	19780103	US 1976-669995		19760324
PRIORITY APPLN. INFO.:			LU 1973-34590	A	19731227
			US 1974-531344	A2	19741210

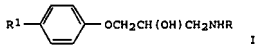
IT 57725-58-3P 57725-59-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57725-58-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[[3-[4-(ethoxymethyl)phenoxy]-2-hydroxypropyl]amino]ethyl]- (9CI) (CA INDEX NAME)



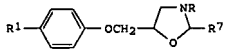
RN 57725-59-4 HCAPLUS
CN 2-Furanmethanol, α-[2-[[2-hydroxy-3-[4-(methoxymethyl)phenoxy]propyl]amino]ethyl]- (9CI) (CA INDEX NAME)



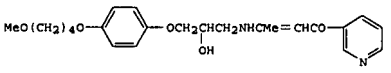
L8 ANSWER 95 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI



I



II



IV

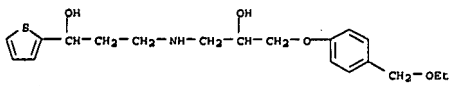
AB The title compds. I [R = CR2:CHCOR3, CHR2CH2CH(OH)R3 (R2 = H, Me; R3 = an aromatic or quasi-aromatic 5- or 6-membered monocyclic ring, with 1 or 2 N, O, and (or) S atoms, which can be substituted with 1 or more Me groups, and connected via a C atom); R1 = alkoxymethyl, alkoxyalkoxy, hydroxyalkoxy, NHCONR4R5 (R4 and R5 = Ph, alkyl, alkenyl, cycloalkyl; NR4R5 = a saturated 5- or 6-membered heterocyclic group, which may have O or S as an addnl. heteroatom), and contain C1-4 alkyl or alkoxy groups, C3-4 alkenyl groups, and C5-7 cycloalkyl groups] as well as their aldehyde condensation products and acid addition salts, were prepared by treating 4-R1C6H4OCH2CH(OH)CH2NH2 with RR6 (R as above, R6 = halo, OH, OK, ONa) and the obtained I, if necessary, converted with R7CHO (R7 = H, C1-4 alkyl) into oxazolidines II or with an acid into acid addition salts. Thus, e.g., 4-MeO(CH2)4OC6H4OCH2CH(OH)CH2NH2 (III) in EtOH was treated with nicotinoylacetone and the mixture treated with 1 drop HCO2H and refluxed 3 h to give 78% the nicotinoylvinylamino ether IV. Nicotinoylacetone was prepared by dropwise treatment of KOCMe3 in C6H6 with EtOAc and 3-acetylpyridine at 10° and keeping the mixture 24 h at room temperature III was prepared by heating 4-HOC6H4OCH2Ph with MeO(CH2)4Br in Me2CO with excess K2CO3, hydrogenolysis of the formed 4-MeOC6H4OR8 (V, R8 = CH2Ph), treating the phenol V (R = H) with epichlorohydrin, and ammonolysis of the resulting glycidyl ether V (R = glycidyl). An addnl. 54 I and 1 oxazolidine derivative were prepared Selected I had ED50 0.003-0.093 mg/kg (dog) as β1-receptor inhibitors and ED50 1.02-15.59 mg/kg (dog) as β2-receptor inhibitors [vs. 0.238 and 26.505 for 4-

L8 ANSWER 95 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Me2CHNHCH2CH(OH)CH2OC6H4NHAc] and are useful in treating arrhythmia and other heart disorders.

ACCESSION NUMBER: 1978:89525 HCAPLUS
DOCUMENT NUMBER: 88:89525
TITLE: 1-Phenoxy-3-aminopropan-2-ol derivatives and their acid addition salts
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Austrian, 20 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

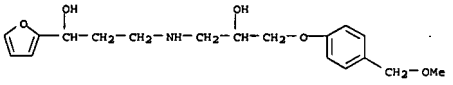
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
AT 339306	B	19771010	AT 1974-10166		19741219
AT 7410166	A	19770215			
US 4088764	A	19780509	US 1974-531344		19741210
FI 7403631	A	19750628	FI 1974-3631		19741216
NO 7404530	A	19750630	NO 1974-4530		19741216
SE 7415761	A	19750630	SE 1974-15761		19741216
DK 7406547	A	19750825	DK 1974-6547		19741216
DD 117071	A5	19751220	DD 1974-183198		19741219
ZA 7408082	A	19760128	ZA 1974-8082		19741219
SU 559643	A3	19770525	SU 1974-2085461		19741219
SU 598557	A3	19780315	SU 1974-2085234		19741219
HU 171726	B	19780328	HU 1974-CA376		19741219
CA 1047512	A1	19790130	CA 1974-216421		19741219
US 4066768	A	19780103	US 1976-669995		19760324
PRIORITY APPLN. INFO.:			LU 1973-34590	A	19731227
			US 1974-531344	A2	19741210

IT 57725-58-3P 57725-59-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57725-58-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[[3-[4-(ethoxymethyl)phenoxy]-2-hydroxypropyl]amino]ethyl]- (9CI) (CA INDEX NAME)

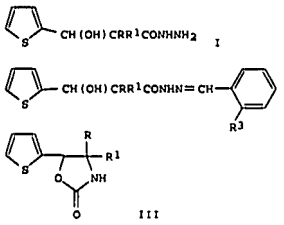


RN 57725-59-4 HCAPLUS
CN 2-Furanmethanol, α-[2-[[2-hydroxy-3-[4-(methoxymethyl)phenoxy]propyl]amino]ethyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 95 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 96 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI

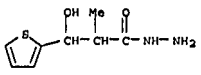


AB The hydrazides I (R = Me, Et, R1 = H (2 stereoisomers of each), R = R1 = Me) were prepared from the corresponding esters. Treatment of I with 2-R3C6H4CHO gave the hydrazones II (R3 = H, OH). I were treated with HNO2 to give oxazolidinones III.

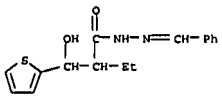
ACCESSION NUMBER: 1977:89661 HCAPLUS
DOCUMENT NUMBER: 86:89661
TITLE: Preparation of 5-(2-thienyl)-2-oxazolidinone
AUTHOR(S): Zhelyazkov, L.; Mavrova, A.
CORPORATE SOURCE: Bulg.
SOURCE: Khimiya i Industriya (1922-1988) (1976), 48(7), 291-3
CODEN: KINSAP; ISSN: 0368-5764
DOCUMENT TYPE: Journal
LANGUAGE: Bulgarian
OTHER SOURCE(S): CASREACT 86:89661

IT 61948-44-5P 61948-45-6P 61948-54-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, oxazolidinones from)

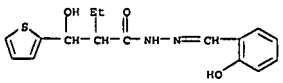
RN 61948-44-5 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, hydrazide (9CI) (CA INDEX NAME)



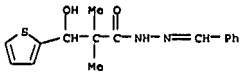
L8 ANSWER 96 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)



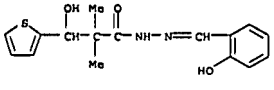
RN 61948-49-0 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, [(2-hydroxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)



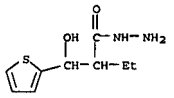
RN 61948-50-3 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α,α-dimethyl-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)



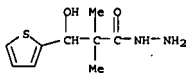
RN 61948-51-4 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α,α-dimethyl-, [(2-hydroxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)



L8 ANSWER 96 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 61948-45-6 HCAPLUS
CN 2-Thiophenepropanoic acid, α-ethyl-β-hydroxy-, hydrazide (9CI) (CA INDEX NAME)

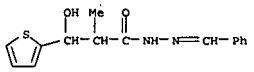


RN 61948-54-7 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α,α-dimethyl-, hydrazide (9CI) (CA INDEX NAME)

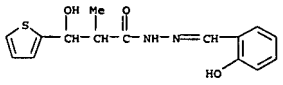


IT 61948-46-7P 61948-47-8P 61948-48-9P
61948-49-0P 61948-50-3P 61948-51-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 61948-46-7 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)



RN 61948-47-8 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-α-methyl-, [(2-hydroxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)



RN 61948-48-9 HCAPLUS

L8 ANSWER 97 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB 1-Phenoxy-3-amino-2-propanols 4-RC6H4OCH2CH(OH)CH2NHR1 (I; R = alkoxymethyl, alkoxyalkoxy, hydroxyalkoxy, or substituted ureido; R1 = CR2:CHCOR3 or CHR2CH2CHR3OH, where R2 = H or Me, and R3 = a C-bonded 5- or 6-membered heterocyclic ring containing 1 or 2 N, S, and/or O atoms), which were β-receptor blocking agents, were prepared by reacting 4-RC6H4OCH2CH(OH)CH2NH2 with R1X, where X = Br or Cl. Among 56 I thus prepared were (R, R1 given): MeO(CH2)4O, CMe:CHCOR3 (R3 = 3-pyridyl); EtOCH2, 2-(2-thienylcarbonyl)vinyl; EtNHCONH, 2-[(2,4-dimethyl-2-pyrimidinyl)carbonyl]-1-methylvinyl; HOCH2CH2O, 3-(1,5-dimethylpyrazol-4-yl)-3-hydroxy-1-methylpropyl; and morpholinocarboxamido, 3-hydroxy-1-methyl-3-(6-methyl-3-pyridyl)propyl.

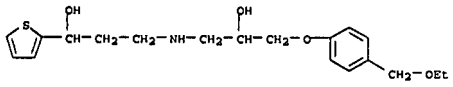
ACCESSION NUMBER: 1976:30897 HCAPLUS
DOCUMENT NUMBER: 84:30897
TITLE: Heterocyclic derivatives of 1-amino-3-phenoxy-2-propanol
INVENTOR(S): Raabe, Thomas; Graewinger, Otto; Scholtholt, Josef; Nitz, Rolf E.; Schraven, Eckhard
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 61 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2458744	A1	19750710	DE 1974-2458744	19741212
NL 7416377	A	19750701	NL 1974-16377	19741216
FR 2255893	A1	19750725	FR 1974-42024	19741219
AU 7476664	A	19760624	AU 1974-76664	19741219
GB 1443135	A	19760721	GB 1974-54911	19741219
ES 433131	A1	19770216	ES 1974-433131	19741219
ES 433132	A1	19770216	ES 1974-433132	19741219
ES 433133	A1	19770216	ES 1974-433133	19741219
CH 602716	A5	19780731	CH 1974-16973	19741219
CH 603584	A5	19780831	CH 1974-16972	19741219
CS 184837	B2	19780915	CS 1974-8779	19741219
CS 184838	B2	19780915	CS 1974-8780	19741219
CS 184850	B2	19780915	CS 1977-1030	19741219
CH 605758	A5	19781013	CH 1974-16974	19741219
RO 69155	A1	19810330	RO 1974-80875	19741219
RO 68397	A1	19810626	RO 1974-80874	19741219
RO 69154	A1	19810730	RO 1974-80873	19741219
JP 50096562	A	19750731	JP 1974-148532	19741226
PRIORITY APPLN. INFO.:			LU 1973-69079 A	19731227

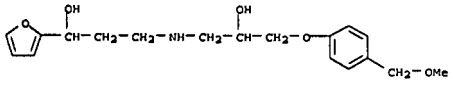
IT 57725-58-3P 57725-59-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 57725-58-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[[3-[4-(ethoxymethyl)phenoxy]-2-hydroxypropyl]amino]ethyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 97 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



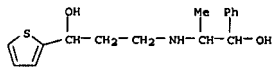
RN 57725-59-4 HCAPLUS
CN 2-Furanmethanol, α-[2-[[2-hydroxy-3-[4-(methoxymethyl)phenoxy]propyl]amino]ethyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 98 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB Thirty-two RCOCH2CH2NHCHMeCHPhOH (I, R = heterocyclyl), useful for treatment of heart disease at 0.1-500 mg oral doses, were prepared by treating 1-norephedrine with acetyl derivative of the appropriate heterocycle.
Thus, a mixture of 12.6 g 2-acetylthiophene, 18.7 g l-norephedrine hydrochloride, 4 g paraformaldehyde in 20 ml Me2CHOH was refluxed with 0.2
mole concentrated HCl for 2 hr to give 17 g I (R = 2-thienyl).
ACCESSION NUMBER: 1975:443189 HCAPLUS
DOCUMENT NUMBER: 83:43189
TITLE: Indole aminoketones
INVENTOR(S): Posselt, Klaus; Thiele, Kurt
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler, Fed. Rep. Ger.
SOURCE: U.S., 8 pp. Continuation-in-part of U. S. 3,658,845 (CA 77:19630a).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

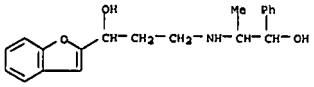
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3859305	A	19750107	US 1971-137575	19710426
US 3514465	A	19700526	US 1967-693138	19671226
US 3658845	A	19720425	US 1970-18300	19700310
PRIORITY APPLN. INFO.:			US 1967-693138	A3 19671226
			US 1970-18300	A2 19700310
			DE 1966-D51910	A 19661230
			DE 1966-D51911	A 19661230

IT 28745-93-9P 28745-94-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-93-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



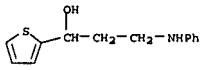
● HCl

L8 ANSWER 98 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 28745-94-0 HCAPLUS
CN 2-Benzofuranmethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

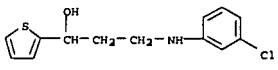


● HCl

L8 ANSWER 99 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB The cyclodehydration of 1-arylamino-3-alkanols I to VII using 70% H2SO4 has been studied. Alkanols I, V and VI give exclusively the rearranged 2,3-disubstituted-1,2,3,4-tetrahydroquinolines VIII; the remaining alkanols give a mixture of 2,3-disubstituted and 3,4-disubstituted 1,2,3,4-tetrahydroquinolines IX. The formation of the rearranged 2,3-disubstituted 1,2,3,4-tetrahydroquinolines is explained on the basis of involvement of N-arylazetidine intermediates. In the case of I and IV the relevant N-arylazetidines X and XI have been isolated.
ACCESSION NUMBER: 1975:409727 HCAPLUS
DOCUMENT NUMBER: 83:9727
TITLE: Synthesis of heterocyclic compounds. XII. Cyclodehydration of 1-arylamino-3-alkanols
AUTHOR(S): Gogte, V. N.; Mukhedkar, V. A.; El Namaky, H. M.; Salama, Mrs. M. A.; Tilak, B. D.
CORPORATE SOURCE: Natl. Chem. Lab., Poona, India
SOURCE: Indian Journal of Chemistry (1974), 12(12), 1234-7
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 83:9727
IT 55439-04-8P 55439-07-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclodehydration of)
RN 55439-04-8 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(phenylamino)ethyl]- (9CI) (CA INDEX NAME)



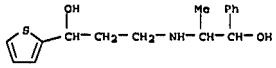
RN 55439-07-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(3-chlorophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 100 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB The ketone (I, R = α-thienyl, α-furyl, 3-pyridyl, 2,4-dimethyl-5-thiazolyl, 3-benzothiophenyl, 3-quinolyl, etc. R1 = H, OMe, R2 = H, F; R3 = H,Cl) were prepared by treating an acetylheterocycle with norephedrine or its derivs. and paraformaldehyde. Thus, 12.6 g 2-acetylthiophene was treated with 18.7 g l-norephedrine-HCl and 4 g paraformaldehyde to give 17 g I(R = 2-thienyl R1 = R2 = R3 = H). Several I were reduced to the corresponding alcs. I increased the cerebral and peripheral blood flow in narcotized dogs.
ACCESSION NUMBER: 1973:136051 HCAPLUS
DOCUMENT NUMBER: 78:136051
TITLE: 2-3-Phenyl-3(hydroxypropylamino) ethyl-3-thienyl ketone
INVENTOR(S): Posselt, Klaus; Thiele, Kurt
SOURCE: U.S., 7 pp. Continuation-in-part of U.S. 3,514,465 (CA 73;7724n).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

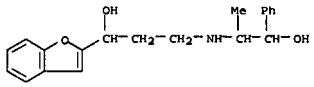
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3715369	A	19730206	US 1970-23455	19700327
DE 1670547	A	19701112	DE 1966-D51911	19661230
DE 1543538	A1	19760205	DE 1966-D51910	19661230
US 3514465	A	19700526	US 1967-693138	19671226
PRIORITY APPLN. INFO.:			DE 1966-D51911 A	19661230
			US 1967-693138 A	19671226
			DE 1966-D51910	19661230

IT 28745-93-9P 28745-94-0P 28745-95-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-93-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



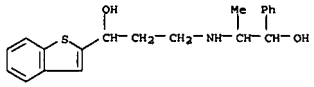
● HCl

L8 ANSWER 100 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 28745-94-0 HCAPLUS
CN 2-Benzofuranmethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



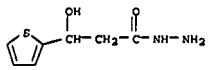
● HCl

RN 28745-95-1 HCAPLUS
CN Benzo[b]thiophene-2-methanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

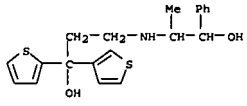
L8 ANSWER 101 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB 2-Ethynylthiophene (I) was prepared by a 4 step sequence which involved the base decomposition of 5-(2-thienyl)-3-nitroso-2-oxazolidone. Metalation of I followed by carbonation and acidification gave 2-thienylpropiolic acid. Thiophene ring metalation was not observed The pKa of I was determined to be 22.4 from competitive metalation expts. on I and phenylacetylene with BuLi.
ACCESSION NUMBER: 1973:43176 HCAPLUS
DOCUMENT NUMBER: 78:43176
TITLE: Synthesis and metalation of 2-ethylnylthiophene
AUTHOR(S): Patrick, Timothy B.; Disher, Joyce M.; Probst, W. J.
CORPORATE SOURCE: Dep. Chem., South Illinois Univ., Edwardsville, IL, USA
SOURCE: Journal of Organic Chemistry (1972), 37(26), 4467-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 20795-13-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20795-13-5 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-, hydrazide (9CI) (CA INDEX NAME)



L8 ANSWER 102 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB The dithienyl carbinols RR1C(OH)CH2CH2-NCHMeCHPhOH (I; R = R1 = 3-thienyl; II; R = 3-thienyl, R1 = 2-thienyl) and their dehydration products RR1C:CR2CH2-NCHMeCHPhOH (III; R = R1 = 3-thienyl; IV, R = 3-thienyl, R1 = 2-thienyl; R2 = H, Me) were prepared Thus, 3-acetylthiophene, HCHO and DL-norephedrine-HCl were refluxed to give DL-β-[(1-phenyl-1-hydroxy-2-propyl)amino]propio-thienone which was treated with 2-thienylmagnesium bromide to give DL-II-HCl. DL-II-HCl was dissolved in CHCl3 and HCl(g) was bubbled through to give DL-IV-HCl (R2 = H).
ACCESSION NUMBER: 1972:564446 HCAPLUS
DOCUMENT NUMBER: 77:164446
TITLE: Dithienylamine derivatives
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: Fr. Demande, 10 pp. Addn. to Fr. 2,042,377 (See Ger. 1,921,453, CA 74;76320c).
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2103478	A6	19720414	FR 1970-34393	19700923
FR 2103478	B2	19740621		
CH 539645	A	19730914	CH 1970-3597	19700311
PRIORITY APPLN. INFO.:			CH 1970-3597 A	19700825
			DE 1969-1921453 A	19690426

IT 37750-25-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)
RN 37750-25-7 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-α-3-thienyl-, hydrochloride (9CI) (CA INDEX NAME)

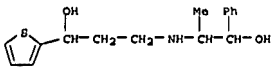


● HCl

L8 ANSWER 103 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB About 30 aminoketones RCOCHR1CH2NHCH2CH(OH)C6H4R2 (I, R = 1,3,5-trimethyl-4-pyrazolyl, 2,4-dimethylthiazolyl, 1,3-dimethyl-4-pyrazolyl, 1-benzyl-2,4-pyrazolyl, thienyl, methylenedioxyphenyl etc., R1 = H, Me, R2 = H, Cl, 3,4-Cl(MeO)) were prepared from 1-norephedrine-HCl and acetyl heterocycles. Thus, 27 g 1,2,3-trimethylacetyl-pyrazole was treated with 33 g 1-norephedrine-HCl, paraformaldehyde, and concentrated HCl to give 14.5 g I (R = 1,3,5-trimethyl-4-pyrazolyl).
ACCESSION NUMBER: 1972:552179 HCAPLUS
DOCUMENT NUMBER: 77:152179
TITLE: Pyrazole and pyrazolinone amino ketones
INVENTOR(S): Posselt, Klaus; Enkheim, Bergen; Thiele, Kurt
PATENT ASSIGNEE(S): deut ge
SOURCE: U.S., 6 pp. Continuation-in-part of U.S. 3,514,465 (CA 76;72214n).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

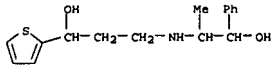
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3686206	A	19720822	US 1970-19511	19700313
DE 1670547	A	19701112	DE 1966-D51911	19661230
DE 1543538	A1	19760205	DE 1966-D51910	19661230
FR 8021	M	19700803	FR 1967-8021	19671229
GB 1203810	A	19700903	GB 1967-1203810	19671229
AT 286978	B	19710111	AT 1967-11809	19671229
PRIORITY APPLN. INFO.:			DE 1966-D51910 A	19661230
			DE 1966-D51911 A	19661230

IT 28745-92-8P 28745-93-9P 28745-94-0P
28745-95-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-92-8 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



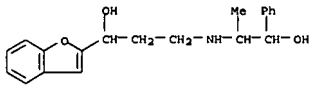
RN 28745-93-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 103 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



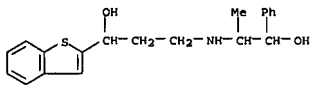
● HCl

RN 28745-94-0 HCAPLUS
CN 2-Benzofuranmethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 28745-95-1 HCAPLUS
CN Benzo[b]thiophene-2-methanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

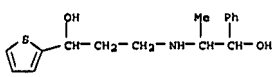


● HCl

L8 ANSWER 104 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB Division of U.S. 3,514,465 (CA73: 77214m). Twenty-four RCOCH2CH2NHCHMeCHPhOH (I,R = heterocycle) and 5 RCH(OH)CH2CH2NHCHMeCHPhOH (R = heterocycle), were prepared Thus, 4-methyl-2-acetylthiazole, norephedrine-HCl, paraformaldehyde, and HCl in iso-PrOH was refluxed 2 hr to give I.HCl (R = 4-methyl-2-thiazolyl).
ACCESSION NUMBER: 1972:419630 HCAPLUS
DOCUMENT NUMBER: 77:19630
TITLE: Benzothiophene amino ketones and amino alcohols
INVENTOR(S): Posselt, Klaus; Thiele, Kurt
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: U.S., 5 pp. Division of U.S. 3,514,465 (CA 73;77214m).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3658845	A	19720425	US 1970-18300	19700310
DE 1670547	A	19701112	DE 1966-D51911	19661230
DE 1543538	A1	19760205	DE 1966-D51910	19661230
FR 8021	M	19700803	FR 1967-8021	19671229
GB 1203810	A	19700903	GB 1967-1203810	19671229
AT 286978	B	19710111	AT 1967-11809	19671229
US 3859305	A	19750107	US 1971-137575	19710426
PRIORITY APPLN. INFO.:			DE 1966-D51910 A	19661230
			DE 1966-D51911 A	19661230
			US 1967-693138 A3	19671226
			US 1970-18300 A2	19700310

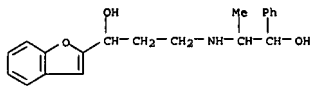
IT 28745-93-9P 28745-94-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-93-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 28745-94-0 HCAPLUS
CN 2-Benzofuranmethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 104 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

L8 ANSWER 105 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB Eight l- or dl-forms of the title compds. RR1CHCH2-CH2NHCHMeCHR2C6H4R3-p.HCl I (R = 2- or 3-thienyl, R1 = 2- or 3-thienyl or Ph, R2 = H or OH, R3
= H, Cl, or F) were prepared by hydrogenation of RR1C:CHCH2NHCHMeCHR2-C6H4R3-
p or RR1C(OH)CH2CH2NHCHMeCHR2C6H4R3-p (II) over Pd/BaSO4. I had LD50 <500
mg/kg orally in mice and were useful for increasing the coronary, cerebral, and peripheral blood flow. Thus, 13 g II maleate (l-form, R = R1 = 2-thienyl, R2 = OH, R3 = H), prepared from EtO2CCH2CH2NHCHMeCH(OH)Ph and 2-thienylmagnesium bromide, was treated with 20% NaOH to give free II,
which was hydrogenated at 6 atmospheric and room temperature in EtOH over 10% Pd/BaSO4
to give 4 g I (l-form, R = R1 = thienyl, R2 = OH, R3 = H).
ACCESSION NUMBER: 1972:419522 HCAPLUS
DOCUMENT NUMBER: 77:19522
TITLE: (3-Thienylpropyl)(1-phenyl-2-propyl)amines
INVENTOR(S): Posselt, Klaus; Offermanns, Heribert
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: Ger. Offen., 25 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2150977	A	19720420	DE 1971-2150977	19711013
DE 2150977	C3	19781116		
AT 308089	B	19730625	AT 1970-9277	19701014
NL 7112892	A	19720418	NL 1971-12892	19710920
NL 165163	B	19801015		
NL 165163	C	19810316		
US 3767675	A	19731023	US 1971-182192	19710920
CH 560211	A5	19750327	CH 1971-13775	19710921
CH 567500	A5	19751015	CH 1974-12693	19710921
AU 7133901	A	19730405	AU 1971-33901	19710927
CS 171163	B2	19761029	CS 1971-6860	19710927
ZA 7106654	A	19720726	ZA 1971-6654	19711005
SU 455540	A3	19741230	SU 1971-1702859	19711005
FI 52581	B	19770630	FI 1971-2817	19711007
FR 2110409	A5	19720602	FR 1971-36274	19711008
FR 2110409	B1	19750207		
BE 773852	A1	19720131	BE 1971-43459	19711012
NO 132592	B	19750825	NO 1971-3741	19711012
DD 95393	A5	19730212	DD 1971-158268	19711013
HU 162962	B	19730528	HU 1971-DE765	19711013
ES 395947	A1	19740901	ES 1971-395947	19711013
DK 131570	B	19750804	DK 1971-4965	19711013
SE 379045	B	19750922	SE 1971-12984	19711013
JP 54041592	B	19791208	JP 1971-81284	19711014

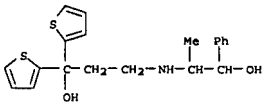
L8 ANSWER 105 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

US 3826838	A	19740730	US 1973-346248	19730330
PRIORITY APPLN. INFO.:			AT 1970-9277	A 19701014
			US 1971-182192	A3 19710920

IT 23978-70-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23978-70-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-α-2-thienyl-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

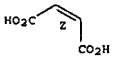
CRN 47419-12-5
CMF C20 H23 N O2 S2



CM 2

CRN 110-16-7
CMF C4 H4 O4

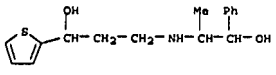
Double bond geometry as shown.



L8 ANSWER 106 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(a), see printed CA Issue.
AB Continuation-in-part of U.S. 3,514,465 (CA 73: 77214n). -Acetylthiophene
was treated with PhCH(OH)CHMeNH2.HCl (I) and paraformaldehyde to give II (R = R1 = R2 = H) (III). About 20 analogs of III were prepared by treatment
of I with paraformaldehyde and acetyl heterocycles (2-acetylfuran, acetylthiazoles, 3-acetylpyridine, acetylpyrazoles, 2-acetylbenzopyran, etc.). Two similar II (R = MeO, R1 = F, R2 = H; R = R1 = H, R2 = Cl) were
prepared III and several of its analogs were reduced to the alcs. The compds. were coronary-dilating agents.
ACCESSION NUMBER: 1972:113205 HCAPLUS
DOCUMENT NUMBER: 76:113205
TITLE: Thiazolyl and pyridyl amino alcohols
INVENTOR(S): Posselt, Klaus; Thiele, Kurt
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: U.S., 6 pp. Continuation-in-part of U.S. 3,514,465 (CA
73:77214n).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

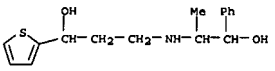
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3631055	A	19711228	US 1970-18279	19700310
PRIORITY APPLN. INFO.:			US 1970-18279 A	19700310

IT 28745-92-8P 28745-93-9P 28745-94-0P
28745-95-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-92-8 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



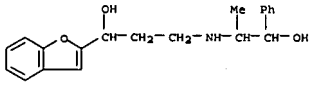
RN 28745-93-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 106 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



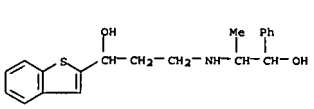
● HCl

RN 28745-94-0 HCAPLUS
CN 2-Benzofuranmethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 28745-95-1 HCAPLUS
CN Benzo[b]thiophene-2-methanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

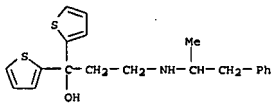
L8 ANSWER 107 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB The title compds. (I) and (II) and their salts with coronary-dilating activity were prepared Thus, the Grignard compound from Mg and 2-bromothiophene in absolute Et2O was refluxed 2 hr with dl-3-(α-methylphenethylamino)-1-(2-thienyl)-1-propanone in Et2O to give dl-I (R = H, 2-position in the thiophene group) (III). Similarly prepared were I (R, position in thiophene, and isomer given): OH, 2, 1; OH, 3, 1. Reaction of 13 g III maleate with HCl in HOAc gave 5 g dl-II.HCl (R = H, 2 position in thiophene). Similarly prepared were II·HCl (R, position in thiophene, and isomer given): OH, 2, 1; OH, 3, 1.
ACCESSION NUMBER: 1971:76320 HCAPLUS
DOCUMENT NUMBER: 74:76320
TITLE: (1,1-Dithienyl-1-hydroxy-3-propyl) and (1,1-dithienyl-1-propen-3-yl)-(1-phenyl-2-propyl)amines
INVENTOR(S): Thiele, Kurt; Posselt, Klaus
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: Ger. Offen., 11 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1921453	A	19701112	DE 1969-1921453	19690426
DE 1921453	C3	19730419		
CH 539645	A	19730914	CH 1970-3597	19700311
CH 542867	A	19731130	CH 1972-15345	19700311
ES 377719	A1	19721016	ES 1970-377719	19700320
FI 50125	B	19750901	FI 1970-800	19700320
NL 7004410	A	19701028	NL 1970-4410	19700326
NO 131675	B	19750401	NO 1970-1422	19700415
GB 1296112	A	19721115	GB 1970-1296112	19700417
SU 457221	A3	19750115	SU 1970-1437303	19700417
BE 749296	A	19701001	BE 1970-749296	19700421
DK 126001	B	19730528	DK 1970-2103	19700423
FR 2042377	A5	19710212	FR 1970-15055	19700424
FR 2042377	B1	19740201		
AT 303716	B	19721211	AT 1970-3775	19700424
AT 307399	B	19730525	AT 1971-2935	19700424
SE 369305	B	19740819	SE 1970-5713	19700424
ES 398738	A1	19740816	ES 1972-398738	19720111
NO 132593	B	19750825	NO 1974-2863	19740808
FI 51193	B	19760802	FI 1975-2248	19750807

PRIORITY APPLN. INFO.: DE 1969-1921453 A 19690426
FI 1970-800 A 19700320

IT 23973-95-7P

L8 ANSWER 107 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 23973-95-7 HCAPLUS
CN 1-Propanol, 3-[(α-methylphenethyl)amino]-1,1-di-2-thienyl- (8CI) (CA INDEX NAME)

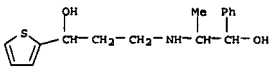


L8 ANSWER 108 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB The title compds. PhCH(OH)CHMeNHC2H4COA (I), where A is a heterocyclic moiety, are stimulants to coronary blood flow. I are prepared by treating PhCH(OH)CHMeNH2 (II) with AcOMe and paraformaldehyde (III) or with AcOCH2CH2Cl or AcOCH:CH2. Thus, 12.6 g 2-acetylthiophene (IV), 18.7 g II.HCl, and 4 g III in 20 ml iso-PrOH is treated with 0.2 mole concentrated HCl and refluxed 2 hr to give the HCl salt of I (A = 2-thienyl) (V), m. 191-2°. II (1.5 g) and 2.7 g 2-thienyl vinyl ketone in 60 ml Et2O gave, after 0.5 hr, V, m. 118-20°. 2-(β-Chloropropionyl)thiophene (5.2 g), 4.5 g II, and 4 g Et3N in Me2NCHO gave V after 1 hr. Similarly, using the first method, are prepared the following I (A and m.p. HCl salt given): 2-furanyl, 186-7°; 2-(4-methylthiazolyl), 197-9°; 4-antipyryl, 206-8°; 3-pyridyl, 187-9°; 5-(2,4-dimethylthiazolyl), 208-10°; 5-(4-methyl-2-hydroxythiazolyl), 209-10°; 2-coumaronyl, 199-200°; 3-thionaphthenyl, 200-21°; 3-(1-methylindolyl), 194-5°; 3,4-methylenedioxyphenyl, 195-7°; 4-(1,3-dimethylpyrazolyl), 196°; 3-quinolyl, 205-6°; 4-isoquinolyl, 208°; 3-(1,2,4-trimethyl-5-carbethoxypyrrolyl), 178-80°; 6-(benzo-1,4-dioxanyl), 201°; 2-(benzo-1,4-dioxanyl), 178°; 4-(2-benzyl-10-hydroxydecahydroisoquinolyl), 182-3°; 2-(5-nitrofuryl), 210°; 4-(1,3,5-trimethylpyrazolyl), 191°; 4-(1-benzyl-3,5-dimethylpyrazolyl, 200°; 2-(5-chlorothienyl), 198°. Analogs of I were similarly prepared (reactants and m.p. of HCl salt of product given): (±)-[3,4-P(MeO)C6H3CH(OH)CHMeNH2].HCl, IV, III, 208°; II.HCl, 2-propionylthiophene, III, 208°; (±)-[2-ClC6H4CH(OH)CH2NH2].HCl, IV, III, 158-60°. Other active compds. are prepared by reduction of the carbonyl of I with (iso-PrO)3Al or NaBH4 to give ACH(OH)C2H4NHCHMeCH(OH)Ph (VI). Thus were prepared VI (A and m.p. of HCl salt given): 2-(4-phenylthiazolyl), 178-81°; 2-thenyl, 152-3°; 2-coumaranyl, 210-15°; 2-thionaphthenyl, 167-70°.
ACCESSION NUMBER: 1970:477214 HCAPLUS
DOCUMENT NUMBER: 73:77214
TITLE: Coronary dilating 2-(3-phenyl-3-hydroxy-2-propylamino)ethyl heterocyclic ketones
INVENTOR(S): Posselt, Klaus; Enkheim, Bergen; Thiel, Kurt
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

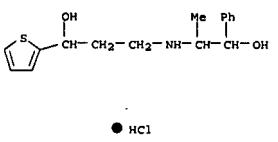
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3514465	A	19700526	US 1967-693138	19671226
DE 1670547	A	19701112	DE 1966-D51911	19661230
DE 1543538	A1	19760205	DE 1966-D51910	19661230
FR 8021	M	19700803	FR 1967-8021	19671229
GB 1203810	A	19700903	GB 1967-1203810	19671229
AT 286978	B	19710111	AT 1967-11809	19671229
US 3715369	A	19730206	US 1970-23455	19700327

L8 ANSWER 108 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
US 3859305 A 19750107 US 1971-137575 19710426
PRIORITY APPLN. INFO.: DE 1966-D51910 A 19661230
DE 1966-D51911 A 19661230
US 1967-693138 A 19671226
US 1970-18300 A2 19700310

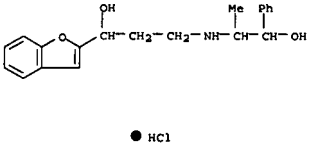
IT 28745-92-8P 28745-93-9P 28745-94-0P
28745-95-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28745-92-8 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 28745-93-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

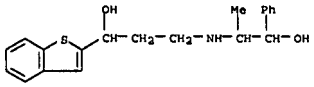


RN 28745-94-0 HCAPLUS
CN 2-Benzofuranmethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



RN 28745-95-1 HCAPLUS

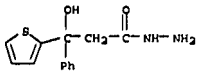
L8 ANSWER 108 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN Benzo[b]thiophene-2-methanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



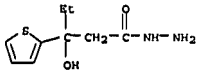
● HCl

L8 ANSWER 109 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB Throughout this abstract, Q = 2-thienyl. Reformatskii reaction gave 40-6% R1R2C(OH)CH2CO2Et (R1, R2 and m.p. given): Ph, Q, 52-3°; Q, Q, 48°; and Ph, 2-thiazolyl, 95°. The following R1R2C(OH)CH2CONHNH2 were prepared in 60-83% yields by stirring the ester with 80% N2H4.H2O, in C5H5N, 4 hr with cooling (same data given): Ph, Q (I), 139-40°; Ph, 2-thiazolyl, 167°; Et, Q, 112°; 2-thiazolyl, Q, 169-70°; and Q, Q, 111-13°. I was converted into QPhC(OH)CH2CONHN:CHR (R and m.p. given): Et, 171°; Ph 215°; furyl, 184°; and Q, 189°. The following R1PhC(OH)CH2CONHNHR (R1 = Q unless otherwise noted) were prepared by N-alkylation and acylation of the hydrazides or hydrogenation (R and m.p. given): Et (II), 167°; iso-Pr, 116° (HCl salt); Bu, 114° (HCl salt); Bu (R1 = 2-thiazolyl), 165°; pentyl, 170°; QCH2, 184°; furfuryl, 161°; PhCH2, 169-70°; Ac, 187°; Bz, 233°; p-MeC6H4SO2, 163°; and CH2SO3Na, 167° (prepared by refluxing the hydrazide, 12 hr, with aqueous HOCH2SO3Na). Similarly prepared were R1PhC:CHCONHNHR.HCl (R1, R, and m.p. given): Ph, H, 169°; Q, H (III), 181°; and Q, Bu, 89-90°. PhMgBr and QCOCO2Et gave 73% QPhC(OH)CO2Et, b3 142-4°, converted into QPhC(OH)CONHNH2, m. 128-30°. Also prepared was QPhCHCH2CONHNH2.HCl, m. 160°. Hypoglycemic activity was tested with oral doses of 100 mg/kg to fasting rabbits. The hydrazides, e.g. I, were fairly active and the activity was enhanced by N-alkylation or conversion to hydrazones. Acryloylhydrazides, e.g. III, also had high activity, which was lowered by saturation of the double bond. II and III were most active, but had somewhat high toxicity in mice.
ACCESSION NUMBER: 1970:476963 HCAPLUS
DOCUMENT NUMBER: 73:76963
TITLE: Hypoglycemics. II. Hypoglycemic activity of β,β-disubstituted β-hydroxypropanohydrazide derivatives
AUTHOR(S): Kurihara, Tozaburo; Takeda, Hideo; Ito, Hideo; Sagawa, Keiko
CORPORATE SOURCE: Japan
SOURCE: Annual Report of the Tohoku College of Pharmacy (1969), No. 16, 39-51
CODEN: TYKNAQ; ISSN: 0495-7342
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
IT 29101-06-2P 29101-08-4P 29101-10-8P
29101-11-9P 29101-12-0P 29101-13-1P
29101-14-2P 29101-15-3P 29101-16-4P
29101-18-6P 29101-19-7P 29101-20-0P
29101-21-1P 29101-23-3P 29122-81-4P
29122-82-5P 29625-32-9P 29625-33-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29101-06-2 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, hydrazide (8CI) (CA INDEX NAME)

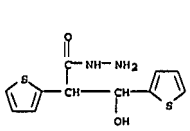
L8 ANSWER 109 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



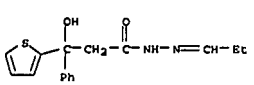
RN 29101-08-4 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-ethyl-, hydrazide (8CI) (CA INDEX NAME)



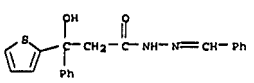
RN 29101-10-8 HCAPLUS
CN Hydracrylic acid, 3,3-di-2-thienyl-, hydrazide (8CI) (CA INDEX NAME)



RN 29101-11-9 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, propylidenehydrazide (8CI) (CA INDEX NAME)

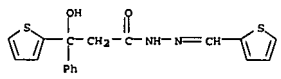


RN 29101-12-0 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, benzylidenehydrazide (8CI) (CA INDEX NAME)

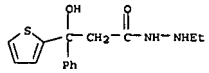


RN 29101-13-1 HCAPLUS

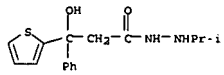
L8 ANSWER 109 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Thiophenehydracrylic acid, β-phenyl-, (2-thenylidene)hydrazide (8CI) (CA INDEX NAME)



RN 29101-14-2 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, 2-ethylhydrazide (8CI) (CA INDEX NAME)

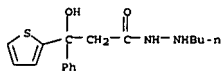


RN 29101-15-3 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, 2-isopropylhydrazide monohydrochloride (8CI) (CA INDEX NAME)



● HCl

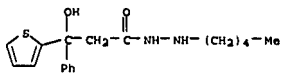
RN 29101-16-4 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, 2-butylhydrazide monohydrochloride (8CI) (CA INDEX NAME)



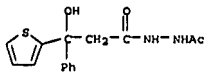
● HCl

RN 29101-18-6 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, 2-pentylhydrazide (8CI) (CA INDEX NAME)

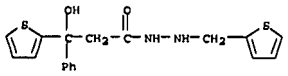
L8 ANSWER 109 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



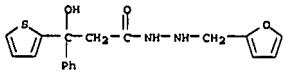
RN 29101-19-7 HCAPLUS
CN Hydrazine, 1-acetyl-2-(β-hydroxy-β-2-thienylhydrocinnamoyl)- (8CI) (CA INDEX NAME)



RN 29101-20-0 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, 2-(2-thenyl)hydrazide (8CI) (CA INDEX NAME)

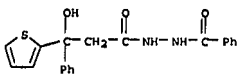


RN 29101-21-1 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, 2-furfurylhydrazide (8CI) (CA INDEX NAME)

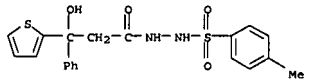


RN 29101-23-3 HCAPLUS
CN Hydrazine, 1-(β-hydroxy-β-2-thienylhydrocinnamoyl)-2-(p-tolylsulfonyl)- (8CI) (CA INDEX NAME)

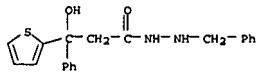
L8 ANSWER 109 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



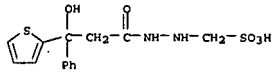
L8 ANSWER 109 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 29122-81-4 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, 2-benzylhydrazide (8CI) (CA INDEX NAME)

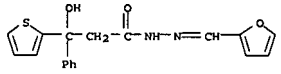


RN 29122-82-5 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, 2-(sulfomethyl)hydrazide, monosodium salt (8CI) (CA INDEX NAME)



● Na

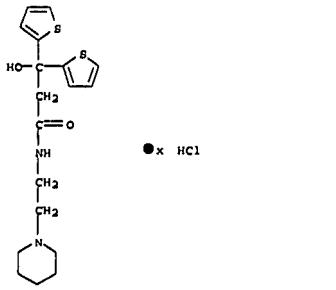
RN 29625-32-9 HCAPLUS
CN 2-Thiophenehydracrylic acid, β-phenyl-, furfurylidenehydrazide (8CI) (CA INDEX NAME)



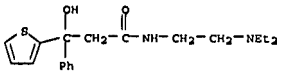
RN 29625-33-0 HCAPLUS
CN Hydrazine, 1-benzoyl-2-(β-hydroxy-β-2-thienylhydrocinnamoyl)- (8CI) (CA INDEX NAME)

L8 ANSWER 110 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB A mixture of 15 g. 2-thienyl Ph ketone, 16 g. EtO2CCH2Br, and 50 ml. C6H6, after addition of 6 g. Zn and 0.5 g. Cu, was refluxed 3 hrs. to give 12 g. Et 3-phenyl-3-thienyl-3-hydroxypropionate (I), m. 53° (EtOH). Hydrolysis of I by refluxing with 10% NaOH 3 hrs. gave 46% 3-phenyl-3-thienyl-3-hydroxypropionic acid (II), m. 170° (EtOH). Similarly prepared were the following R1R2C(OH)CH2CO2Et (R1, R2, m.p., and m.p. of the free acid given): thienyl, thienyl (IIa), 48°, 131°; 2-pyridyl, Ph, 46°, 171°; 2-thiazolyl, Ph, 95°, 128°; 2-furyl, Ph, 32°, 155°; and 2-pyrrolyl, Ph, 75-6°, 147°. Refluxing 5 g. II with 50 ml. 10% HO2CCO2H afforded 3.4 g. 3-thienyl-3-phenylacrylic acid (III), m. 113° (EtOH-Me2CO). Heating 2 g. Et2NCH2CH2Cl and 2 g. III in 10 ml. iso-PrOH gave 1.5 g. dimethylaminoethyl 3-phenyl-3-thienyl-3-hydroxypropionate-HCl, m. 156° (absolute EtOH). Similarly prepared were the following R3R4C(OH)CH2-CO2CHR5CH2R6-HCl (R3, R4, R5, R6, and m.p. given): thienyl, Ph, H, Me2N, 158-9°; thienyl, Ph, H, piperidino, 165°; thienyl, Ph, H, morpholino, 158-60°; thienyl, thienyl, H, Et2N, 140-1°; thienyl, thienyl, H, piperidino, 147-9°; 2-thiazolyl, Ph, H, piperidino, 151-2°; and thienyl, Ph, Me, Et2N; and also the following R7R8C:CHCO2CHR9CH2R10-HCl (R7, R8, R9, R10, and m.p. given): thienyl, phenyl, H, Et2N, 136-8°; thienyl, Ph, H, piperidino, 152°; thienyl, Ph, H, morpholino, 149°; thienyl, Ph, Me, Et2N, 124-6°; and thienyl, thienyl, H, Et2N, 129°. Heating 2 g. IIa and 2 g. (2-piperidinoethyl)amine (IV) at 140-50° 3 hrs. afforded 2.4 g. N-(2-piperidinoethyl)-3,3-dithienyl-3-hydroxypropionamide-HCl, m. 156°. Similarly prepared were the following R11R12C(OH)CH2CONHCH2CH 2R13-HCl (R11, R12, R13, and m.p. given): thienyl, Ph, Et2N, 98°; thienyl, Ph, piperidino, 166°; thienyl, Ph, morpholino, 116°; thienyl, thienyl, Et2N, 128-30°; and thienyl, thienyl, Bu2N, syrup. II (2 g.) in 10 ml. C6H6 was warmed with 6 g. SOCl2 2 hrs. After removal of excess SOCl2, 2 g. IV in 5 ml. C6H6 was added and the mixture kept at room temperature 5 hrs. to give 1.8 g. N-(2-piperidinoethyl)-3-phenyl-3-thienylacrylamide-HCl, m. 112°. Topical local anesthetic activities of the compds. are described.
ACCESSION NUMBER: 1969:512757 HCAPLUS
DOCUMENT NUMBER: 71:112757
TITLE: Local anesthetics. XXI. Derivatives of 3,3-disubstituted-3-hydroxypropionic acids
AUTHOR(S): Kurihara, Tozaburo; Kumamoto, Ko; Takeda, Hideo
CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai, Japan
SOURCE: Annual Report of the Tohoku College of Pharmacy (1967), No. 14, 51-8
CODEN: TYKNAQ; ISSN: 0495-7342
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 23997-30-0P 23997-31-1P 23997-32-2P
23997-33-3P 23997-34-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23997-30-0 HCAPLUS
CN Hydracrylamide, N-(2-piperidinoethyl)-3,3-di-2-thienyl-, hydrochloride (8CI) (CA INDEX NAME)

L8 ANSWER 110 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

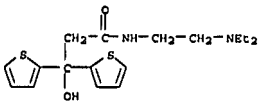


RN 23997-31-1 HCAPLUS
CN 2-Thiophenehydracrylamide, N-[2-(diethylamino)ethyl]-β-phenyl-, hydrochloride (8CI) (CA INDEX NAME)

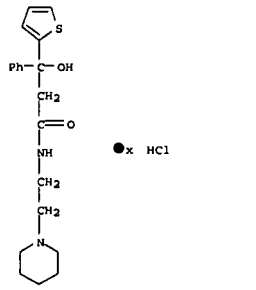


RN 23997-32-2 HCAPLUS
CN 2-Thiophenehydracrylamide, β-phenyl-N-(2-piperidinoethyl)-, hydrochloride (8CI) (CA INDEX NAME)

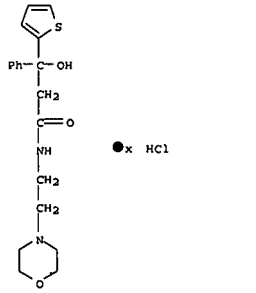
L8 ANSWER 110 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 110 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

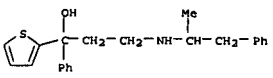


RN 23997-33-3 HCAPLUS
CN 2-Thiophenehydracrylamide, N-(2-morpholinoethyl)-β-phenyl-, hydrochloride (8CI) (CA INDEX NAME)



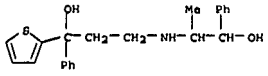
RN 23997-34-4 HCAPLUS
CN Hydracrylamide, N-[2-(diethylamino)ethyl]-3,3-di-2-thienyl-, hydrochloride
(8CI) (CA INDEX NAME)

L8 ANSWER 111 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB HOCRR1-(CH2)2NHCHR2CHR3C6H4R4-p (I) (R = 2-thienyl, R1 = Ph) were prepared by
treating Bz(CH2)2NHCHR2R3C6H4R4-p with 2-thienyl-lithium or 2-thienylmagnesium bromide, or by treating RCO-(CH2)2NHCHR2CHR3C6H4R4-p (R
= 2-thienyl) (II) with PhLi or PhMgBr. Treatment of II with 2-thienylmagnesium bromide gave I (R = R1 = 2-thienyl). Treatment of I with P and iodine or HCl-HOAc gave RR1C:CHCH2NHCHR2CHR3C6H4R4-p (III). The following compds. (R = 2-thienyl) were prepared (R1, R2, R3, R4, salt I,
m.p., and m.p. III hydrochloride given): Ph, Me, H, H, hydrochloride, 190°, 174°; Ph, Me, H, Cl, maleate, 145-6°,
193-4°; Ph, Me, H, MeO, hydrochloride, 160-1°,
183-4°; Ph, Me, OH, H, hydrochloride, 195-7°, 204°;
Ph, Me, OH, OH, malonate, 184-5°, -; Ph, H, OH, Cl, malonate,
157-8°, 200-1°; Ph, H, OH, MeO, maleate, 166-7°, -;
2-thienyl, Me, OH, H, maleate, 137-8°, 188-9°. I and III increased coronary blood flow in Langendorff prepns. by 69-180% at doses of 10 γ. Some of them also increased the amplitude of contraction by 80-150%. Relacement of Ph by 2-thienyl in I slightly decreased the coronary activity, while in III it had no effect.
ACCESSION NUMBER: 1969:491188 HCAPLUS
DOCUMENT NUMBER: 71:91188
TITLE: Thienyl alkylanimes with coronary blood flow increasing actions
AUTHOR(S): Thiele, Kurt; Posselt, K.; Gross, A.; Schuler, A. W.
CORPORATE SOURCE: Lab. Arzneimittelforsch., Chemiewerk Homburg, Homburg,
Fed. Rep. Ger.
SOURCE: Chimica Therapeutica (1969), 4(3), 228-33
CODEN: CHTPBA; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: German
IT 2847-93-0P 2847-94-1P 2847-95-2P
6499-05-4P 6499-06-5P 6499-07-6P
23973-93-5P 23973-94-6P 23973-95-7P
23978-67-8P 23978-68-9P 23978-69-0P
23978-70-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2847-93-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



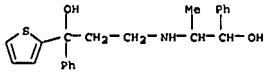
RN 2847-94-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(β-hydroxy-α-

L8 ANSWER 111 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI)
(CA INDEX NAME)

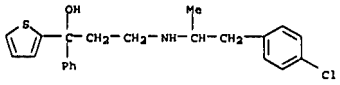


● HCl

RN 2847-95-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(β-hydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)

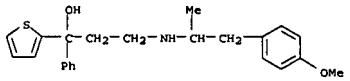


RN 6499-05-4 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(p-chloro-α-methylphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)



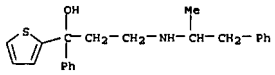
RN 6499-06-5 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(p-methoxy-α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI)
(CA INDEX NAME)

L8 ANSWER 111 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

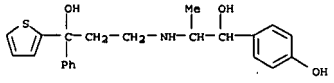
RN 6499-07-6 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)



RN 23973-93-5 HCAPLUS
CN Malonic acid, compd. with α-[2-[(p,β-dihydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl-2-thiophenemethanol (1:1)
(8CI) (CA INDEX NAME)

CM 1

CRN 47524-51-6
CMF C22 H25 N O3 S



CM 2

CRN 141-82-2
CMF C3 H4 O4

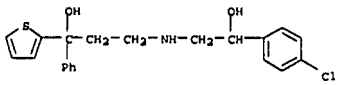
$HO_2C-CH_2-CO_2H$

RN 23973-94-6 HCAPLUS
CN Malonic acid, compd. with α-[2-[(p-chloro-β-

L8 ANSWER 111 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
hydroxyphenethyl)amino]ethyl]-α-phenyl-2-thiophenemethanol (1:1)
(8CI) (CA INDEX NAME)

CM 1

CRN 47470-40-6
CMF C21 H22 Cl N O2 S

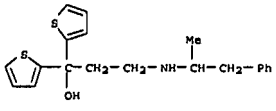


CM 2

CRN 141-82-2
CMF C3 H4 O4

$HO_2C-CH_2-CO_2H$

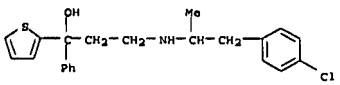
RN 23973-95-7 HCAPLUS
CN 1-Propanol, 3-[(α-methylphenethyl)amino]-1,1-di-2-thienyl- (8CI)
(CA INDEX NAME)



RN 23978-67-8 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(p-chloro-α-methylphenethyl)amino]ethyl]-α-phenyl-, maleate (salt) (1:1) (8CI)
(CA INDEX NAME)

CM 1

CRN 6499-05-4
CMF C22 H24 Cl N O S

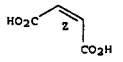


L8 ANSWER 111 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

CRN 110-16-7
CMF C4 H4 O4

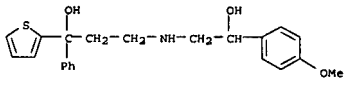
Double bond geometry as shown.



RN 23978-68-9 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(β-hydroxy-p-methoxyphenethyl)amino]ethyl]-α-phenyl-, maleate (1:1) (salt) (8CI)
(CA INDEX NAME)

CM 1

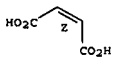
CRN 10489-52-8
CMF C22 H25 N O3 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

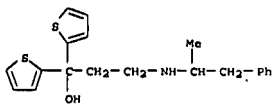


RN 23978-69-0 HCAPLUS
CN 1-Propanol, 3-[(α-methylphenethyl)amino]-1,1-di-2-thienyl-, maleate (1:1) (salt) (8CI) (CA INDEX NAME)

CM 1

CRN 23973-95-7
CMF C20 H23 N O S2

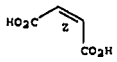
L8 ANSWER 111 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 110-16-7
CMF C4 H4 O4

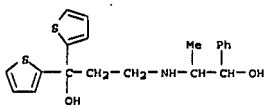
Double bond geometry as shown.



RN 23978-70-3 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(2-hydroxy-1-methyl-2-phenylethyl)amino]ethyl]-α-2-thienyl-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 47419-12-5
CMF C20 H23 N O2 S2

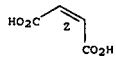


CM 2

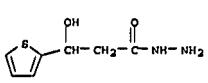
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

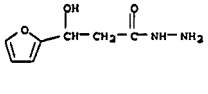
L8 ANSWER 111 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



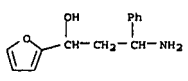
L8 ANSWER 112 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB A number of epinephrine analogs and the corresponding 1-aryl-2-(alkylamino)ethyl chloride hydrochlorides and bromide hydrobromides were prepared. The central intermediates of the syntheses were the 5-aryl-3-alkyl-2-oxazolidones (I), accessible by alkylation of the product obtained using the Reformatskii reaction of an aromatic aldehyde with Et bromoacetate. The compds. were tested for central nervous system activity (mice), spinal depressant activity (mice), smooth muscle relaxation (guinea pig ileum strips), analgesic activity (phenylquinone-treated mice), anorexic activity (mice), local anesthesia (rabbit eye) and antimicrobial activity. Results were tabulated.
ACCESSION NUMBER: 1969:3409 HCAPLUS
DOCUMENT NUMBER: 70:3409
TITLE: Some epinephrine analogs
AUTHOR(S): Bergmann, Ernst D.; Goldschmidt, Zeev
CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of Medicinal Chemistry (1968), 11(6), 1121-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 20795-13-5P 20795-15-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20795-13-5 HCAPLUS
CN 2-Thiophenepropanoic acid, β-hydroxy-, hydrazide (9CI) (CA INDEX NAME)



RN 20795-15-7 HCAPLUS
CN 2-Furanhydracrylic acid, hydrazide (8CI) (CA INDEX NAME)



L8 ANSWER 113 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Reactions of 3-phenyl-5-(2-furyl)-2-isoxazoline (I) are studied; compds. of the general formulas II, III, and IV are prepared I is prepared according to Bianchi et al., (1955). KMnO4 (15 g.) is added to a solution of 3.0 g. I in Me2CO and the mixture kept overnight to give 30% 3-phenyl-2-isoxazoline-5-carboxylic acid, m. 143-4°. A solution of 8.0 g. I in ether is treated with a mixture of 8.0 g. LiAlH4 in ether and the mixture refluxed 20 hrs. to give 96% 3-phenyl-3-amino-1-(2-furyl)-1-propanol (V), m. 95-6°; methiodide m. 158.5-9.5°. A solution of 0.5 g. V in dilute HCl is treated at 0° with an aqueous solution of NaNO2 to give 0.17 g. III [R = H, R1 = PhCH(OH)CH2CH(OH)], m. 121-2°, which is also prepared by the reduction of III (R = H, R1 = AcCH2CO) (VI) with NaBH4. A mixture of 2 g. I, 4.0 g. chloranil, and xylene is refluxed 5 days to give 15-20% 3-phenyl-5-(2-furyl)isoxazole (VII), m. 78-9° (hexane), which is treated with KMnO4 to give 19.5% IV (R = Ph, R1 = CO2H). An aqueous alc. solution containing 1.0 g. VI and 0.97 g. HONH2.HCl is refluxed 2 hrs. to give 90% mixture containing 75.3% VII (m. 78-9°) and 24.7% IV (R = 2-furyl, R1 = Ph) (VIII) [m. 98-9° (hexane)]; VIII is treated with KMnO4 to give 50% IV (R = CO2H, R1 = Ph), m. 162°. I (0.028 mole) in 80 ml. CCl4 is treated with 0.028 mole N-bromosuccinimide (NBS) in the presence of azodiisobutyronitrile to give 55% II (R = 5-bromo-2-furyl) (IX), m. 86°. A solution of 1.5 g. IX and 1.3 g. NBS in CCl4 is refluxed 10-15 min. to give 80% IV (R = Ph, R1 = 5-bromo-2-furyl) (X), m. 107-8°. X (6.5 g.) in EtOH is hydrogenated (Raney Ni) to give 48% III (R = BzCH2CO, R1 = Br) (XI), m. 87.5-8.5°. XI is treated with HONH2.HCl to give a mixture containing 70% X (m. 107-8°) and 24% IV (R = 5-bromo-2-furyl, R1 = Ph) [m. 137° (hexane)]. III (R = H, R1 = PhC:CCO) is treated with HONH2.HCl to give 78% VIII and <5% VII. VIII is treated with NBS to give X. Uv data are given.
ACCESSION NUMBER: 1968:427306 HCAPLUS
DOCUMENT NUMBER: 69:27306
TITLE: Furyl isoxazoline derivatives
AUTHOR(S): Bianchi, Giorgio; Cogoli, Augusto; Gandolfi, Remo
CORPORATE SOURCE: Univ. Pavia, Pavia, Italy
SOURCE: Gazzetta Chimica Italiana (1968), 98(1), 74-84
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Italian
IT 19986-68-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19986-68-6 HCAPLUS
CN Furfuryl alcohol, α-(β-aminophenethyl)- (8CI) (CA INDEX NAME)



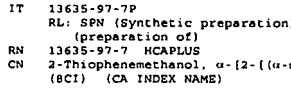
L8 ANSWER 113 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L8 ANSWER 114 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB N-(m-Arylalkyl)dialkylamines, RAr(CH2)nNR1R2, where R is a phenyl or naphthyl group, 2-thienyl, or 2-furyl, are prepared Thus, 15.1 g. 3-phenyl-3-hydroxypropylamine is treated with 14.5 g. PhCH2COMe and the product treated with 1.5 g. NaBH4 to give 25 g. N-(3-phenyl-3-hydroxypropyl)-N-(1-methyl-2-phenylethyl)amine-HCl (I), m. 158-60°. I (25 g.) is treated with 40 ml. SOCl2 to give 30 g. N-(3-phenyl-3-chloropropyl)-N-(1-methyl-2-phenylethyl)-amine-HCl (II), m. 152-4°. II (10 g.) is treated with 30-40 ml. C6H6 in the presence of 8 g. AlCl3 to give 12 g. N-(3,3-diphenylpropyl)-N-(1-methyl-2-phenylethyl)amine-HCl, m. 190-2°, (MeOH). Also prepared are (m.p. given): N-(3,3-diphenylpropyl)dimethylamine-HCl, 186-8°; N-(3,3-diphenylpropyl)-diethylamine-HCl, 172-4°; N-(3,3-diphenylpropyl)dipropylamine-HCl, 146-8°; N-(3,3-diphenylpropyl)dibutylamine-HCl, 120-2°; N-(3,3-diphenylpropyl)morpholine-HCl, 202-4°; N-[3-phenyl-3-(p-tolyl)propyl]dimethylamine-HCl, 182-4°; N-[3-phenyl-3-(3,4-dimethylphenyl)propyl]dimethylamine-HCl, 178-80°; N-[3-phenyl-3-(2,4-dimethylphenyl)propyl]dimethylamine-HCl, 184-6°; N-[3-(p-tolyl)-3-(2,4-dimethylphenyl)propyl]dimethylamine-HCl, 138-40°; N-[3-phenyl-3-(p-fluorophenyl)propyl]dimethylamine-HCl, 180-2°; N-[3-propyl-3-(p-tolyl)propyl]diethylamine-HCl, 156-8°; N-[3-phenyl-3-(p-fluorophenyl)propyl]diethylamine-HCl, 138-40°; N-[3-phenyl-3-(p-fluorophenyl)propyl]piperidine-HCl, 158-60°; N-[3-(p-tolyl)-3-(p-fluorophenyl)propyl]piperidine-HCl, 140-2°; N-[3-phenyl-3-(p-fluorophenyl)propyl]pyrrolidine-HCl, 159-61°; N-[3-phenyl-3-(p-fluorophenyl)propyl]morpholine-HCl, 198-200°; N-[3-(p-tolyl)-3-(p-fluorophenyl)propyl]morpholine-HCl 180-2°; N-[3,3-diphenylpropyl]-1-azacycloheptane-HCl, 190-2°; N-[3-phenyl-3-(p-tolyl)propyl]-1-azacycloheptane-HCl, 184-6°; N-[3-phenyl-3-(p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 206-8°; N-[3-phenyl-3-(p-tolyl)propyl]-N-(2-phenyl-1-methylethylamine-HCl, 178-80°; N-(3-(p-ethylchlorophenyl)-3-(p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 200-2°. N-[3-(p-tolyl)-3-(p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 176-8°; N - [3-phenyl-3-(3,4-dimethylphenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 176-8°; N-[3-phenyl-3-(2,4-dimethylphenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 165-7°; N-[3-(p-fluorophenyl)-3-(p-tolyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 206-8°; N-(3,3-dimethylphenyl)-N-(2-phenyl-1-methylethyl)-N-methylamine-HCl, 168-70°; N-[3-(p-tolyl)-3-phenylpropyl]-N-(2-phenyl-1-methylethyl)-N-methylamine-HCl, 140-2°; N-[3,3-di(p-tolyl)propyl]-N-(2-phenyl-1-methylethyl)-N-methylamine-HCl, 141-3°; N-[3-phenyl-3-(p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)-N-methylamine-HCl, 164-6°; N-[3-(p-chlorophenyl)-3-(methyl-p-fluorophenyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 170-2°; N-(3,3-diphenylpropyl)-N-(1-phenylethyl)amine-HCl, 204° and 205°; N-[3-phenyl-3-(p-tolyl)propyl]-N-(1-phenylethyl)amine-HCl, 196-8°; N-(3-m-tolyl)-3(p-tolyl)propyl]-N-(1-phenylethyl)amine-HCl, 188-90°; N-[3-phenyl-3-(p-fluorophenyl)propyl]-N-(1-phenylethyl)amine-HCl, 206-8°; N-(3,3-diphenylpropyl)-N-(1-phenylpropyl)amine-HCl, 214-16°; N-[3-phenyl-3-(p-fluorophenyl)propyl]-N-(1-phenylpropyl)amine-HCl, 218-20°; N-(3-phenyl-3-(p-tolyl)propyl]-N-(1-phenylpropyl)-amine-

L8 ANSWER 114 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
HCl, 208-10°; N-[3-(m-tolyl)-3-(p-tolyl)propyl]-N-(1-phenylpropyl)amine-HCl, 188-90°; N-[2,2-diphenylethyl]dimethylamine-HCl, 203-5°; N-[2-phenyl-2-(p-fluorophenyl)-ethyl]dimethylamine-HCl, 208-10°; N - (2,2-diphenylethyl)-diethylamine-HCl, 116-18°; N - (2,2-diphenylethyl)piperidine-HCl, 180-2°; amine maleate m. 140-2°; N-(2,2-diphenylethyl)morpholine-HCl, 211-13°; N-[2-phenyl-2-(p-fluorophenyl)ethyl]piperidine-HCl, 178-80°; amine maleate m. 152-4°; N-[2-phenyl-2-(p-fluorophenyl)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 160-2°; N-(2-phenyl-2-(p-tolyl)-ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 168-70°; N-[2-(m-tolyl)-2-(p-tolyl)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 156-8°; N-[2-(0-tolyl)-2-(p-tolyl)ethyl]-N-(2-phenyl-1-methylethyl]amine maleate, 152-4°; N-[2-phenyl-2-(p-chlorophenyl)ethyl]-N-(2-phenyl-1-methylethyl]amine maleate, 163-5°; N-(2,2-diphenylethyl)-N-methyl-N-(2-phenyl-1-methyl-ethyl)amine maleate, 134-6°; N-[2-phenyl-2-(p-fluorophenyl)-ethyl]-N-methyl-N-(2-phenyl-1-methylethyl)amine maleate, 140-2°; N-[2-phenyl-2-(p-tolyl)ethyl]-N-methyl-N-(2-phenyl-1-methylethyl]amine maleate, 146-8°; N-(2,2-diphenylethyl)-N-(1-phenylethyl)amine maleate, 138-40°; N-[2-phenyl-2-(p-fluorophenyl)ethyl]-N-(1-phenylethyl)amine maleate, 130-2°; N-[2-phenyl-2-(p-tolyl)ethyl]-N-(1-phenylethyl)amine maleate, 128-30°; N-[2-(m-tolyl)-2-(p-tolyl)ethyl]-N-(1-phenylethyl]-amine maleate, 128-30°; N-(2,2-diphenylethyl)-N-(1-phenylethyl]-amine maleate, 133-5°; N-[2-phenyl-2-(p-fluorophenyl)-ethyl]-N-(1-phenylpropyl]amine maleate, 130-2°; N-(2,2-diphenylethyl)-N-benzylamine-HCl, 210-12°; N-[2-phenyl-2-(p-tolyl)ethyl]-N-benzylamine-HCl, 203-5°; α-N-(3,3-diphenyl-propyl)morpholine-HCl, 196-8°.; β-N-(3,3-diphenylpropyl]morpholine-HCl,190-2°; N-[3-phenyl-3-(2-thienyl)propyl]dimethyl-amine-HCl, 132-4°; N-[3-phenyl-3-(2-thienyl)propyl]diethyl-amine-HCl, 123-5°; N-[2-phenyl-2-(2-thienyl)ethyl]diethyl-amine-HCl, 128-30°; N-[3-phenyl-3-(2-thienyl)propyl]piperidine maleate, 118-20°; N-[3-phenyl-3-(2-thienyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 178-80°; N-[2-phenyl-2-(2-thienyl)ethyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 144-6°; N-[3-phenyl-3-(2-furyl)propyl]dimethylamine maleate, 134-6°; N-[3-phenyl-3-(2-furyl)propyl]diethylamine maleate, 130-2°; N-[2-phenyl-2-(2-furyl)ethyl]diethylamine maleate, 122-4°; N-[3-phenyl-3-(2-furyl)propyl]piperidine maleate, 128-30°; N-[2-phenyl-2-(2-furyl)ethyl]morpholine maleate, 136-8°; N-[3-phenyl-3-(2-furyl)propyl]-N-(2-phenyl-1-methylethyl)-amine maleate, 124-6°; N-[2-phenyl-2-(2-fury)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 118-20°; N-[3-phenyl-3-(1-naphthyl)propyl]dimethylamine-HCl, 154-6°, amine picrate m. 166-8°; N-[3-phenyl-3-(1-naphthyl)propyl]diethylamine-HCl, 138-40°, amine picrate m. 150-2°; N-[2-phenyl-2-(1-naphthyl)ethyl]diethylamine-HCl, 130-2°; N-[3-phenyl-3-(1-naphthyl)propyl]piperidine-HCl, 128-30°; N-[2-phenyl-2-(1-naphthyl)ethyl]morpholine-HCl, 154-6°; N-[3-phenyl-3-(1-naphthyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 188-90°; N-[3-phenyl-3-(2-naphthyl)propyl]dimethylamine-HCl, 140-2°; N-[3-phenyl-3-(2-naphthyl)propyl]diethylamine-HCl, 136-8°; N-[3-phenyl-3-(2-naphthyl)propyl]piperidine maleate, 128-30°; N-[3-phenyl-3-(5,6,7,8-tetrahydro-1-naphthyl)propyl]diethyl-amine-HCl, 98-110°; N-[2-phenyl-2-(5,6,7,8-tetrahydro-1-naphthyl)ethyl]diethylamine-HCl, 10° (-108°) [sic]; N-[3-phenyl-3-(5,6,7,8-tetrahydro-1-naphthyl)propyl]piperidine maleate, 112-14°; N-[2-phenyl-2-(5,6,7,8-tetrahydro-1-naphthyl)ethyl]-

L8 ANSWER 114 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
piperidine maleate, 118-20°; N-[2-phenyl-2-(5,6,7,8-tetrahydro-1-naphthyl)ethyl]morpholine-HCl, 110-12°; N-[3-phenyl-3-(5,6,7,8-tetrahydro-1-naphthyl)ethyl]morpholine-HCl, 104-6°; N-[3-phenyl-3-(5,6,7,8-tetrahydro)propyl] - N - (2-phenyl-1-methylethyl)amine-HCl, 160° (turbid) and 182-4°; N-[3-phenyl-3-(2-naphthyl)propyl]-N-(2-phenyl-1-methylethyl)-amine-HCl, 140-2°; N-[3-hydroxy-3-(2-thienyl)propyl]dimethyl-amine, 69-71°, HCl salt m. 158-60°; N-[3-chloro-3-(2-thienyl)-propyl]dimethylamine, 42-4°; N-[3-hydroxy-3-(2-thienyl)-propyl]diethylamine, 38-40°; N-[3-hydroxy-3-(2-thienyl)propyl]piperidine-HCl, 160-2°; N-[3-hydroxy-3-(2-thienyl)propyl]-N-(2-phenyl-1-methylethyl)amine, 36-8°, ketone HCl salt m. 164-6°; N-[3-hydroxy-3-(1-naphthyl)propyl]dimethylamine-HCl, 144-6°; N-[3-hydroxy-3-(1-naphythyl)propyl]diethylamine-HCl, 132-4°; N-[3-hydroxy-3-(1-naphthyl)propyl]piperidine, 112-14°; N-[3-chloro-3-(1-naphthyl)propyl]piperidine, 98-100°, HCl salt m. 178-80°; N-[3-hydroxy-3-(1-naphthyl)-propyl]-N-(2-phenyl-1-methylethyl)amine, 34-6°; N-[3-chloro-3-(1-naphthyl)propyl]-N-(2-phenylpropyl)amine-HCl, 152-4°; N-[3-hydroxy-3-(2-naphthyl)propyl]dimethylamine, 90-2°; N-[3-chloro-3-(2-naphthyl)propyl]dimethylamine-HCl, >240°; N-[3-hydroxy-3-(2-naphthyl)propyl]-N-(2-phenyl-1-methylethyl)-amine-HCl, 170-2°, ketone HCl salt m. 158-60°; N-[3-chloro-3-(2-naphthyl)propyl]-N-(2-phenyl-1-methylethyl)amine-HCl, 154-6°; 3-phenyl-3-chloropropylamine-HCl, 110-12°; 3,3-diphenylpropylamine-HCl, 204-6°; N-(3-hydroxy-3-phenylpropyl)piperidine, 54-6°; N-(3-phenyl-3-chloropropyl)piperidine-HCl, N-(3,3-diphenylpropyl]piperidine-HCl, 208-10°; N-(2,2-diphenylethyl)-N-(2-phenyl-1-methylethyl)amine, 168-70°; N-[2-pheny-2-(p-toly)ethyl]-N-(2-phenyl-1-methylethyl)amine maleate, 166-8°; N-[N-hydroxy-3-(2-naphthyl)propyl]diethylamine, 34-6°; N-[3-chloro-3-(2-naphthyl)propyl]piperidine, 80-2°; N-[3-chloro-3-(2-naphthyl)propyl]piperidine-HCl, >250°.

ACCESSION NUMBER: 1967:46160 HCAPLUS
DOCUMENT NUMBER: 66:46160
TITLE: New method for preparation of diaryl alkyl amines
AUTHOR(S): Klosa, Josef
CORPORATE SOURCE: Privatlab., Berlin-Zehlendorf, Germany
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1966), 34(5-6), 312-34
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: German
IT 13635-97-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 13635-97-7 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-(8CI) (CA INDEX NAME)



L8 ANSWER 114 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L8 ANSWER 115 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

AB Compds. of structure (I) were prepared and found to have coronary vasodilating and pos. inotropic effects (guinea pigs). Thus to a 5° solution of 2-thienyllithium (prepared from 77 g. BuLi and 49 g. thiophene in iso-C5H12) was added 177 g. 2-[(3-phenyl-3-oxopropyl)amino]-3-phenyl-3-hydroxypropane in Et2O, the mixture stirred 1 hr., decomposed with aqueous NH4Cl, and the Et2O phase separated to give 2-[[3-phenyl-3-(2-thienyl)-3-hydroxypropyl]amino]-3-phenyl-3-hydroxypropane (II), b0.02 200-45°; hydrochloride, m. 203° (iso-PrOH), II was also prepared via the Grignard reagent from 2-bromothiophene, m. 72-3° (petr. ether-Et2O). Reaction of 16 g. [2-(1-phenyl-1-hydroxyisopropylamino)ethyl]2-thienylketone-HCl with PhLi (from 48 g. PhBr and 2.8 Li) afforded 10 g. 2-[[3-phenyl-3-(2-thienyl)-3-hydroxypropyl]amino]-3-phenyl-3-hydroxypropane (III), m. 73°; hydrochloride m. 203° (iso-PrOH). III was also prepared via the phenyl Grignard reagent; L.D.50 509 mg./kg., orally (mice). Refluxing 56 g. α-[[1-(4-hydroxyphenyl)-1-hydroxy-2-propyl]amino]propiophenone-HCl with 2-thiophene Grignard reagent (from 146.5 g. 2-bromothiophene) in tetrahydrofuran 6 hrs. and then treating with malonic acid gave 31 g. 2-[[3-phenyl-3-(2-thienyl)-3-hydroxypropyl]amino] - 3 - (4 - hydroxyphenyl) 3 - hydroxypropane malonate, m. 184-5° (iso-PrOH); L.D.50 1750 mg./kg. Also synthesized were: [3-phenyl-3-(2-thienyl)-3-hydroxypropyl][2-(4-chlorophenyl)-2-hydroxyethyl]amine malonate, m. 157-8° (MeCOEt), L.D.50 3400 mg./kg.; and 2-[[3phenyl - 3 - (2 - thienyl) - 3 - hydroxypropyl] amino] (4 - methoxy-phenyl)-1-hydroxyethane malonate, m. 166-7° (EtOH). These compds. compared favorably with, or were superior to papaverine and 2-ethyl-3-(3,5-diiodo-4-hydroxybenzoyl)benzofuran with respect to rate and amplitude of coronary flow (tested on guinea pigs).

ACCESSION NUMBER: 1966:482157 HCAPLUS
DOCUMENT NUMBER: 65:82157
ORIGINAL REFERENCE NO.: 65:15328e-h
TITLE: Thiophene compounds
INVENTOR(S): Thiele, Kurt; Posselt, Klaus
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

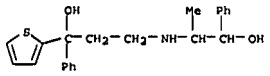
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1219038		19660616	DE 1962-D40471	19621208
PRIORITY APPLN. INFO.:			DE	19621208

IT 2847-94-1P, 2-Thiophenemethanol, α-[2-[(β-hydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride
2847-95-2P, 2-Thiophenemethanol, α-[2-[(β-hydroxy-

L8 ANSWER 115 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

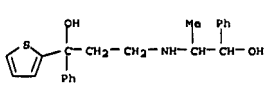
α-methylphenethyl)amino]ethyl]-α-phenyl- 10489-52-8P, 2-Thiophenemethanol, α-[2-[(β-hydroxy-p-methoxyphenethyl)-amino]ethyl]-α-phenyl- 14480-71-8P, 2-Thiophenemethanol, α-[2-[(p,β-dihydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl-, malonate 14480-72-9DP, Malonic acid, compd. with α-[2-[(p-chloro-β-hydroxyphenethyl)amino]ethyl]-α-phenyl-2-thiophenemethanol, cyclic acetals 14480-72-9P, 2-Thiophenemethanol, α-[2-[(p-chloro-β-hydroxyphenethyl)amino]ethyl]-α-phenyl-, malonate 14480-73-0P, 2-Thiophenemethanol, α-[2-[(β-hydroxy-p-methoxyphenethyl)-amino]ethyl]-α-phenyl-, maleate 23973-93-5P, Malonic acid, compds. with α-[2-[(p,β-dihydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl-2-thiophenemethanol
RL: PREP (Preparation)
(prepn. of)

RN 2847-94-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(β-hydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

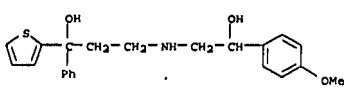


● HCl

RN 2847-95-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(β-hydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)



RN 10489-52-8 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(β-hydroxy-p-methoxyphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)



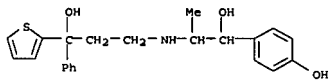
RN 14480-71-8 HCAPLUS
CN Malonic acid, compd. with α-[2-[(p,β-dihydroxy-α-

L8 ANSWER 115 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

methylphenethyl)amino]ethyl]-α-phenyl-2-thiophenemethanol (8CI) (CA INDEX NAME)

CM 1

CRN 47524-51-6
CMF C22 H25 N O3 S



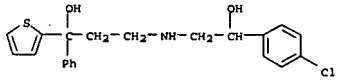
CM 2

CRN 141-82-2
CMF C3 H4 O4

RN 14480-72-9 HCAPLUS
CN Malonic acid, compd. with α-[2-[(p-chloro-β-hydroxyphenethyl)amino]ethyl]-α-phenyl-2-thiophenemethanol (8CI) (CA INDEX NAME)

CM 1

CRN 47470-40-6
CMF C21 H22 Cl N O2 S



CM 2

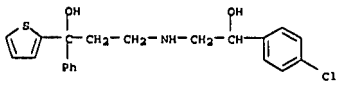
CRN 141-82-2
CMF C3 H4 O4

RN 14480-72-9 HCAPLUS
CN Malonic acid, compd. with α-[2-[(p-chloro-β-hydroxyphenethyl)amino]ethyl]-α-phenyl-2-thiophenemethanol (8CI) (CA INDEX NAME)

L8 ANSWER 115 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

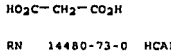
CM 1

CRN 47470-40-6
CMF C21 H22 Cl N O2 S



CM 2

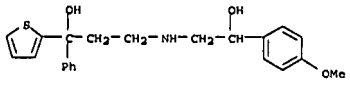
CRN 141-82-2
CMF C3 H4 O4



RN 14480-73-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(β-hydroxy-p-methoxyphenethyl)amino]ethyl]-α-phenyl-, maleate (8CI) (CA INDEX NAME)

CM 1

CRN 10489-52-8
CMF C22 H25 N O3 S

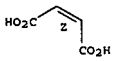


CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

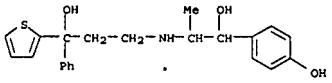
L8 ANSWER 115 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 23973-93-5 HCAPLUS
CN Malonic acid, compd. with α-[2-[(p,β-dihydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl-2-thiophenemethanol (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 47524-51-6
CMF C22 H25 N O3 S



CM 2

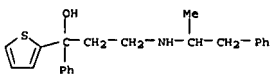
CRN 141-82-2
CMF C3 H4 O4

L8 ANSWER 116 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB Addition to Ger. 1,194,424 (See Fr. 1,338,098, CA 60, 2896e). The title compds. (I) are prepared by addition of 2-thienyl magnesium bromide (II) to β-aralkylaminopropiophenones. II, from 32.6 g. 2-thienyl bromide (III) and 4.8 g. Mg in 100 ml. absolute Et2O, was treated with 60.6 g. PhCH2CHMeNHCH2CH2COPh.HCl in 500 ml. Et2O, then with 50 g. NH4Cl in 150 ml. H2O and the mixture neutralized with HCl in iso-PrOH to give 47 g. I. HCl (X = H) (Ia.HCl), m. 190° (iso-PrOH). Similarly prepared were 12.8 g. (I, X = Cl) (Ib), b0.4 250-2°, Ib.HCl m. 145-6° (iso-PrOH), from 3.5 g. Mg, 23.6 g. III, and 23 g. p-ClC6H4CH2CHMeNHCH2CH2COPh.HCl; and 28 g. I. HCl (X = OMe) (Ic.HCl), m. 160-1° (2:1 EtOAc-EtOH), from 6.2 g. Mg, 41 g. III, and 42 g. p-MeOC6H4CH2CHMeNHCH2CH2COPh.HCl. PhLi from 2.3 g. Li and 48 g. PhBr in 200 ml. absolute Et2O, treated with 31 g. 2-C4H3SCOCH2CH2NHCHMeCH2Ph.HCl (C4H3 = thienyl) in 300 ml. absolute Et2O, gave 13 g. Ia, b1 225-35°. These products are central nervous system stimulants.
ACCESSION NUMBER: 1966:412208 HCAPLUS
DOCUMENT NUMBER: 65:12208
ORIGINAL REFERENCE NO.: 65:2224a-c
TITLE: 2-Thienyl(phenylaralkyl)(aminoethyl)carbinols
INVENTOR(S): Thiele, Kurt
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: 2 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1213851		19660407	DE	19621207
PRIORITY APPLN. INFO.:			DE	19621207

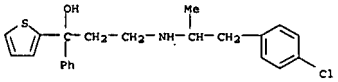
IT 2847-93-0P, 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride
6499-05-4P, 2-Thiophenemethanol, α-[2-[(p-chloro-α-methylphenethyl)amino]ethyl]-α-phenyl- 6499-06-5P, 2-Thiophenemethanol, α-[2-[(p-methoxy-α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride
6499-07-6P, 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl- 6506-56-5P, 2-Thiophenemethanol, α-[2-[(p-chloro-α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 2847-93-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

L8 ANSWER 116 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

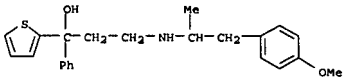


● HCl

RN 6499-05-4 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(p-chloro-α-methylphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)

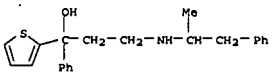


RN 6499-06-5 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(p-methoxy-α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



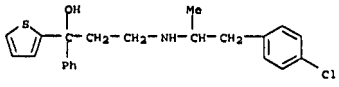
● HCl

RN 6499-07-6 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)



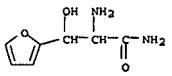
RN 6506-56-5 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(p-chloro-α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

L8 ANSWER 116 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

L8 ANSWER 117 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB Et β-furylglycidate (I) was prepared in 60% yield from furfural, ClCH2CO2Et, and EtONa by the Darzens method with the improvement of adding to the reaction mixture 20-30 mg. each of hydroquinone and S as the stabilizers. Et α-chloro-β-furylacrylate, m. 44°, b2 88°, and possessing fungicidal properties was isolated as a by-product. A mixture of 13.65 g. I and 50 ml. absolute EtOH saturated at 0° with NH3 was sealed in an ampul and left to react at room temperature overnight to prepare the amide (II) of β-furylserine in 53% yield. II, m. 177-9°, was also prepared in the same yield when a saturated aqueous solution of NH3 was substituted for the alc. solution Furfural was isolated from the oxidation of II with Pb(OAc)4 in HOAc. dl-erythro-β-Furylserine (III), decomposing at 250°, Rf 0.25 (on paper with ascending 200:150:25:25 BuOH-H2O-Me2CO-NH3) with ir bands at 1522 and 1622 cm.-1, glycine, and an unidentified amino compound, Rf 0.20 (same conditions), were obtained as a 45:4:51 mixture by boiling 1 g. II and 1.8 g. Ba(OH)2 in 25 ml. H2O until the evolution of NH3 had ceased. III separated by paper partition chromatography was identified by comparison with dl-threo- and dl-erythro-β-furylaerine which were prepared as a 97: 2: 1 mixture with glycine by the method of Hayes and Gever (CA 45, 8504a). Hence, II was assumed to have the erythro configuration.
ACCESSION NUMBER: 1966:19065 HCAPLUS
DOCUMENT NUMBER: 64:19065
ORIGINAL REFERENCE NO.: 64:3448f-h
TITLE: Reaction of ethyl β-furylglycidate with ammonia
AUTHOR(S): Kastron, Ya. A.; Hillers, S.
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1965), (4), 471-7
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT 4505-07-1P, 2-Furanhydracrylamide, α-amino-
RL: PREP (Preparation)
(preparation of)
RN 4505-07-1 HCAPLUS
CN 2-Furanhydracrylamide, α-amino- (7CI, 8CI) (CA INDEX NAME)

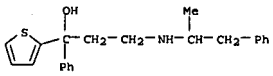


L8 ANSWER 118 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB Addition to Belg. 628,104 (see Fr. 1.338,098, CA 60, 2896e). Compds. of the general formula I are prepared and can be used as coronary dilators. Thus, the Grignard reagent prepared from 4.8 g. Mg and 32.6 g. 2-bromothiophene is treated with 60.6 g. PhCH(OH)CH2CH2NHCHMeCH2Ph.HCl to give 67% 2-[N-(3-phenyl-3-thienyl-3-hydroxy-1-propyl)amino]-1-phenylpropane (II), HCl salt m. 190°. Also prepared is 2-[N-(3-phenyl-3-thienyl-3-hydroxy-1-propyl)amino]-1-phenyl-1-hydroxypropane, b0.02 200-45°, HCl salt m. 203° (iso-PrOH). A solution of 40 g. II in 400 ml. HOAc is treated 20 min. with HCl gas and refluxed 1 hr. to give 2-[N-(3-phenyl-3-thienyl-1-propen-1-yl)amino]-1-phenylpropane, HCl salt m. 174° (iso-PrOH). Similarly prepared are the following I (X, Ar, and m.p. HCl salt given): H, p-ClC6H4, 193-4° (iso-PrOH); OH, Ph, 204° (iso-PrOH).
ACCESSION NUMBER: 1965:90789 HCAPLUS
DOCUMENT NUMBER: 62:90789
ORIGINAL REFERENCE NO.: 62:16194e-g
TITLE: 2-[N-(3-Phenyl-3-thienyl-1-propen-1-yl)amino]-1-phenylpropanes
INVENTOR(S): Thiele, Kurt; Posselt, Klaus
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: 11 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 640572		19640316	BE	
DE 1217967			DE	
FR AD84866			FR	
PRIORITY APPLN. INFO.:			DE	19621130

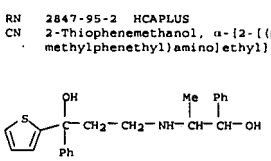
IT 2847-93-0P, 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride
2847-95-2P, 2-Thiophenemethanol, α-[2-[(β-hydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 2847-93-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

L8 ANSWER 118 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

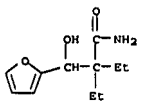


● HCl

RN 2847-95-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(β-hydroxy-α-methylphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 119 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB C6H6 (5 ml.) was distilled from a mixture of 8 g. BrCEt2CONH2 and 17 ml. C6H6, the mixture cooled, 4.4 g. BzH, 2.7 g. finely cut Zn foil, and 4 ml. absolute ether added, at 20° iodine crystals were added, and the mixture was refluxed 2 hrs., cooled, and treated with 42 ml. 10% AcOH for 15 min. to give 77% PhCH(OH)CEt2CONH2, 134-5°, Et ester, b9 155-6°. Similarly were prepared the following RCH(OH)CR21CONH2 (R, R1, % yield, and m.p. given): p-MeOC6H4, Et, 77.2, 147.5-48°; p-tolyl, Et, 77.7, 125-6°; furfuryl, Et, 36.8, 99-100.5°; o-MeOC6H4, Et, 34.3, 126-7°; o-EtOC6H4, Et, 38.2, 116-17°; 3,4-(MeO)2C6H3, Et, 34.1, 137-8°; p-tolyl, Me, 72.7, 164.5-65°; p-Me2NC6H4, Me, 56.3, 163.5-4.5°.
ACCESSION NUMBER: 1964:90516 HCAPLUS
DOCUMENT NUMBER: 60:90516
ORIGINAL REFERENCE NO.: 60:15769g-h,15770a
TITLE: Preparation of amides of α,α-dialkyl-β-hydroxy-β-arylpropionic acids by a modification of the Reformatskii reaction
AUTHOR(S): Sivertseva, A. V.
SOURCE: Trudy Leningradskogo Khimiko-Farmatsevticheskogo Instituta (1962), (14), 7-12
From: Ref. Zh., Khim. 1963, Abstr. No. 17Zh105.
CODEN: TLKFAD; ISSN: 0371-9235
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 91340-70-4P, 2-Furanhydracrylamide, α,α-diethyl-
RL: PREP (Preparation)
(preparation of)
RN 91340-70-4 HCAPLUS
CN 2-Furanhydracrylamide, α,α-diethyl- (7CI) (CA INDEX NAME)

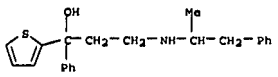


L8 ANSWER 120 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB Novel aralkylamines containing a thienyl group are prepared by the addition of organometallic compds. to the appropriate ketone and subsequent reduction of the hydroxyl group formed, or by the reductive condensation of an aralkyl ketone with the properly substituted amine. Thus, to a cooled solution of 12.8 g. BuLi in 20 ml. Et2O is added dropwise at 15° 8.4 g. thiophene, the mixture kept 0.5 hr., cooled to 5°, 26.7 g. 2-[N-[(3-phenyl-3-oxopropyl)]amino]-1-phenylpropane in Et2O added, the mixture stirred 1 hr., decomposed with NH4Cl with cooling, and the Et2O layer separated and worked up to give 2-[N-(3-phenyl-3-(thien-2-yl)-3-hydroxypropyl]amino]-1-phenylpropane (I), b2 235-41°; HCl salt m. 190°. A mixture of 38.7 g. I, 62 ml. AcOH, 0.4 g. red P, 1.2 g. I, and 1.2 ml. H2O is refluxed 2.5 hrs. and the mixture worked up and distilled to give 2-[N-[3-phenyl-3-(thien-2-yl)propyl]amino]-1-phenylpropane (II), b0.5 280-300°; HCl salt m. 174°. The compds. and their salts are stimulants and have a dilating action on the coronaries.
ACCESSION NUMBER: 1964:16589 HCAPLUS
DOCUMENT NUMBER: 60:16589
ORIGINAL REFERENCE NO.: 60:2896d-f
TITLE: Aralkylamines
PATENT ASSIGNEE(S): Deutsche Gold- und Silber-Scheideanstalt vorm. Roessler
SOURCE: 14 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1338098		19630920	FR 1962-913907	19621030
BE 628104			BE	
DE 1194424			DE	
GB 970445			GB	
US 3251858		1966	US	
PRIORITY APPLN. INFO.:			DE	19611110

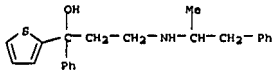
IT 2847-93-0P, 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride
6499-07-6P, 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 2847-93-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

L8 ANSWER 120 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 6499-07-6 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[(α-methylphenethyl)amino]ethyl]-α-phenyl- (7CI, 8CI) (CA INDEX NAME)

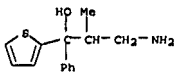


L8 ANSWER 121 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB Novel aminopropanols are prepared by treating the hydrochloride of an aliphatic or alicyclic secondary amine (I) in the presence of HCHO with 2-propionylthiophene (II) and condensing the Mannich base thus obtained with an arylmagnesinm halide. Their diastereoisomers are obtained by treating I with an arylpropanone according to Mannich and by subsequently condensing the Mannich base with a 2-thienylmagnesium halide. Dehydration of the 2 isomers leads to the same aminopropene. The compds. are useful intermediates and exhibit powerful spasmolytic action. A mixture of 0.1 mole II, 0.1 mole Me2NH.HCl (III), 0.12 mole paraformaldehyde (IV), and 20 ml. absolute EtOH is heated on the steam bath 2-3 hrs., cooled, filtered, the EtOH evaporated from the filtrate under reduced pressure, 50 ml. H2O added, the aqueous solution washed with Et2O, made alkaline, the oily Mannich base extracted with Et2O, the Et2O solution of 3'-dimethyl-amino-2'-methyl-2-propionylthiophene refluxed with excess PhMgBr, the mixture hydrolyzed with ice-HCl, the Et2O layer decanted, the aqueous solution and the precipitate made alkaline, and the solid base filtered and dried to give α-dl-3-dimethylamino-2-methyl-1-phenyl-1-(2-thienyl)propanol (V), m. 73° (alc.-H2O). V is dissolved in the calculated amount of aqueous HCl, the solution taken to dryness in vacuo, and the residue taken up in a mixture of MeOH and EtOAc to yield the hydrochloride of V, m. 248°. The B-isomer of V, m. 79° (hydrochloride m. 240-4°), is prepared by treating 3-dimethylamino-2-methylpropionylbenzene (obtained from propiophenone, III, and IV) with thienylmagnesinm iodide. To a solution of 30 g. V (or its B-isomer) in 50 ml. AcOH is added 50 ml. AcOH containing 10 g. gaseous HCl, the mixture taken to dryness in vacuo, and the residue taken up in EtOAc and dioxane to give the hydrochloride of 3-dimethylamino-2-methyl-1-phenyl-1-(2-thienyl)propene, m. 198-9°. Similarly are prepared the following 3-substituted 2-methyl-1-phenyl-1-(2-thienyl)propanols (substituent, m.p. of α-isomer, m.p. of the hydrochloride of the α-isomer, m.p. of B-isomer, m.p. of the hydrochloride of the B-isomer, m.p. of the hydrochloride of the corresponding propene, given): dl-N-pyrrolidino, 122°, 198°, 95°, 240°, 142°; dl-N-piperidino, 106°, 202°, --, -- , 169°; dl-N-morpholino, 101°, 190°, --, --, 160°.
ACCESSION NUMBER: 1963:3239 HCAPLUS
DOCUMENT NUMBER: 58:3239
ORIGINAL REFERENCE NO.: 58:507c-f
TITLE: N-Derivatives of phenylthienylpropanol and phenylthienylpropene
INVENTOR(S): Parthouat, Jean M.
PATENT ASSIGNEE(S): Institut de Serotherapie Hemopoietique
SOURCE: 4 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

L8 ANSWER 121 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1218631		19600511	FR	19581219
PRIORITY APPLN. INFO.:			FR	19581219

IT 856940-14-2, 2-Thiophenemethanol, α-[1-(aminomethyl)ethyl]-α-phenyl- (deriva.)
RN 856940-14-2 HCAPLUS
CN 2-Thiophenemethanol, α-[1-(aminomethyl)ethyl]-α-phenyl- (7CI) (CA INDEX NAME)

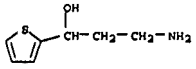


L8 ANSWER 122 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB Derivs. of 1-thienyl-3-aminopropanol were prepared and tested for anticholinergic activity. Thus, 308 cc. cyclohexyl bromide was added to a refluxing suspension of 60.8 g. Mg turnings in 1200 cc. dry ether and refluxed 2 hrs. Dry C6H6 (800 cc.) was added, followed by 62 g. β-diethylaminoethyl 2-thienyl ketone-HCl (I) added over a period of 15 min. at 30-40°. The solvent was distilled until the internal temperature reached 72°, the mixture refluxed 75 min., the mixture cooled to 20°, added to an aqueous solution of 430 g. NH4Cl containing cracked ice, and stirred 5 min. The aqueous acidic layer, resulting from separating and extracting the aqueous layer of the above mixture with Et2O and washing the combined organic layers twice with 200 cc. water containing 25 cc. HCl, was separated, washed with Et2O, made basic with concentrated NH4OH, and extracted twice with C6H6. The residue from the concentrated C6H6 extract was dissolved in 100 cc. Me2CO and treated with 25 cc. 18% alc. HCl at 0°. The solid material which separated was filtered off and recrystd. twice from 40 cc. iso-PrOH to yield 8 g. 1-(2-thienyl)-1-cyclohexyl-3-diethylamino-1-propanol-HCl, m. 181-4°. By substituting 2-(1-piperidyl)ethyl 2-thienyl ketone for I, 1-(2-thienyl)-1-cyclohexyl-3-(1-piperidyl)-1-propanol-HCl (II), m. 222.5-4.0°, was prepared The following compds. were prepared by treating cyclohexylmagnesium bromide with the appropriate thienyl ketone: 1-(2-thienyl)-1-cyclopentyl-3-(4-morpholinyl)-1-propanol; 1-(2-thienyl)-1-cyclohexyl-3-(1-pyrrolidyl)-1-propanol; 1-(3-thienyl)-1-cyclohexyl-3-(1-piperidyl)-1-propanol; 1-(2-thienyl)-1-(4-methylcyclohexyl)-3-dipropylamino-1-propanol; 1-(2-thienyl)-1-cyclopentyl-3-(4-methyl-1-piperidyl)-1-propanol; 1-(3,4-dimethyl-2-thienyl)-1-cyclohexyl-3-(1-piperidyl)-1-propanol. The racemic base of II, m. 75-7°, was prepared by treating an aqueous solution of II with NH4OH, extracting with Et2O, and recrystg. from iso-PrOH. The racemic base of II was treated with d- and l-tartaric acids and the resultant salts treated with NH4OH to yield the levo base of II, m. 81.5-3.5° and the dextro base, m. 82-7°. The levo HCl salt, m. 227°, and the levo quinate, m. 168-70°, of II were prepared by treating the levo base with the appropriate acid. After treating an aqueous solution of II with NH4OH, dissolving the resultant free base in iso-PrOH, and cooling the solution, the precipitated free base was dissolved in MeCN and saturated with MeBr to yield 1-(2-thienyl)-1-cyclohexyl-3(1-piperidyl)-1-propanol methobromide, m. 193.5-5.0°. The compds. prepared were tested for anticholinergic activity and some were found to have considerable atropine-like action.
ACCESSION NUMBER: 1960:74681 HCAPLUS
DOCUMENT NUMBER: 54:74681
ORIGINAL REFERENCE NO.: 54:14268d-i
TITLE: 1-Thienyl-3-aminopropanol derivatives
PATENT ASSIGNEE(S): Sterling Drug Inc.

L8 ANSWER 122 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 826487		19600106	GB 1956-21452	19560711

IT 65653-31-8, 2-Thiophenemethanol, α-(2-aminoethyl)- (deriva.)
RN 65653-31-8 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)- (9CI) (CA INDEX NAME)



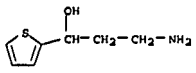
L8 ANSWER 123 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB The title compds., prepared by treating a 2-(aliphatic tertiary amino)lower alkyl ketone with an organometallic compound and hydrolyzing the resulting complex, are antispasmodics with atropinelike action. Cyclohexyl bromide (308 cc.) is added to a refluxing suspension of 60.8 g. Mg turnings in 1200 cc. dry ether, the mixture refluxed 2 hrs., 800 cc. dry C6H6 added, 62 g. β-diethylaminoethyl 2-thienyl ketone-HCl added over 15 min. at 30-40°, a portion of the solvent distilled until the internal temperature reached 72°, the remaining mixture refluxed 75 min., cooled to 20°, added to an aqueous solution of 430 g. NH4Cl containing cracked ice, stirred 5 min., the aqueous layer separated and extracted with ether, the organic layers combined, washed twice with H2O, and extracted with 200 cc. H2O containing 25 cc. concentrated HCl, the aqueous acidic layer separated, washed with ether, made basic with concentrated NH4OH, the basic product extracted twice with C6H6, the C6H6 exts. concentrated, the 39 g. amber oil obtained dissolved in 100 cc. acetone, and 25 cc. 18% HCl in EtOH added to the solution at 0°, yielding 8 g. 1-(2-thienyl)-1-cyclohexyl-3-diethylamino-1-propanol-HCl (I), m. 181-4° (corrected) (iso-PrOH). I is active as an antispasmodic at a dilution of approx. 1:1,400,000 as tested by the modified Magnus method. Similarly prepared are: 1-(2-thienyl)-1-cyclohexyl-3(1-piperidyl)-1-propanol (II).HCl, m. 222.5-4° (corrected) (EtOH) [methobromide, m. 193.5-5° (corrected)]; 1-(2-thienyl)-1-cyclohexyl-2-methyl-3-diethylamino-1-propanol, bl 141-4°, nD25 1.5200-1.5225 (HCl salt, m. 178.5-80°) (prepared from 2-thienyl 2-diethylamino-1-methylethyl ketone, bl 105-10°); 1-(2-thienyl)-1-cyclopentyl-3-(4-morpholinyl)-1-propanol; 1(2-thienyl)-1-cyclohexyl-3-(1-pyrrolidyl)propanol; 1-(3-thienyl)-1-cyclohexyl-3-(1-piperidyl)-1-propanol; 1-(2-thienyl)-1(4-methylcyclohexyl)-3-dipropylamino-1-propanol; 1-(2-thienyl)-1-cyclopentyl-3-(4-methyl-1-piperidyl)-1-propanol; 1-(3,4-dimethyl-2-thienyl)-1-cyclohexyl-3-(1-piperidyl)-1-propanol; and 1-phenyl-1-(2-thienyl)-2-methyl-3-N-piperidyl-1-propanol, m. 103-5-4° (MeOH) (HCl salt, m. 175.5-6°). II.HCl (50 g.) in 250 cc. hot H2O is treated with 15 ml. concentrated NH4OH, the separated semisolid base extracted with ether, the ether removed by distillation, and the residue recrystd. from 50 ml. iso-PrOH, yielding 38 g. racemic II, m. 75-7°. Racemic II (38 g.) and 19 g. d-tartaric acid is dissolved in 400 ml. 90% MeOH, the solution kept at 25° several days, the crystalline precipitate filtered off, washed with a small amount of EtOH, and dried in vacuo, giving 17.3 g. d-II d-bitartrate, m. 90-110°. d-II d-bitartrate (6.5 g.) is dissolved in 100 cc. hot H2O, cooled, made basic with excess NH4OH, the separated base extracted with ether, the ether exts. evaporated, and the residue crystallized from 20 ml. 95% EtOH, giving 2.6 g. d-II, m. 82-7° (corrected), [α]D25 25.3° (0.5%, 95% EtOH). The mother liquors from the separation of d-II d-bitartrate are concentrated to dryness in vacuo, the

L8 ANSWER 123 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
residue (26 g.) dissolved in 200 cc. H2O, made basic with an excess of NH4OH, the sepd. product extd. with ether, the ether exts. concd., and the
residue recrystd. from 95% EtOH, giving 11 g. l-II, m. 72-9°. Further treatment of l-II with l-tartaric acid yields l-bitartrate, m. 90-110°, and treatment with NH4OH yields l-II, m. 81.5-3.5° (cor.) (95% EtOH), [α]D25 -25.5° (0.5%, 95% EtOH). l-II (2.2 g.) in 10 ml. iso-PrOH is treated with 0.55 ml. concd. HCl, the sepd. cryst. material collected by filtration at 5°, washed with cold iso-PrOH and ether, and dried at 60°, giving 2.2 g. l-II.HCl, m. 227°, [α]D25 -36.5° (0.5%, CHCl3), 0° (0.5%, H2O). l-II and 1 equiv. quinic acid yield l-II quinate, m. 168-70°. (Cf. C.A. 49, 6319f).

ACCESSION NUMBER: 1958:113823 HCAPLUS
DOCUMENT NUMBER: 52:113823
ORIGINAL REFERENCE NO.: 52:20205c-i,20206a-b
TITLE: 1-Thienyl-1-cycloalkyl(or aryl)-3-(aliphatic tertiary amino)-1-hydroxy lower alkanes
INVENTOR(S): Ruddy, Arlo W.; Becker, Theodore J.; Tainter, Maurice L.
PATENT ASSIGNEE(S): Sterling Drug Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2837525		19580603	US 1955-521616	19550712

IT 65653-31-8, 2-Thiophenemethanol, α-(2-aminoethyl)- (deriva.)
RN 65653-31-8 HCAPLUS
CN 2-Thiophenemethanol, α-(2-aminoethyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 124 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB The compds., which have antibiotic activity or are intermediates in the synthesis of antibiotics, have the general formula O.CHR.(CH2)2.CHCH(OR1)CH(NHR2)CH2OR3 and are prepared from intermediates in
which the side chain is -COCH(NHR4)CH2OR3 or -COCH2NHR3, where R is H, NO2, halogen, or a low alkyl radical, R1 and R3 are the same or different,
representing H, or acyl groups, and R2 is H, an acyl radical, or 1 equivalent
of an inorg. or organic acid, and R4 is acyl. Dissolve 5-nitro-2-furyl bromomethyl ketone 228 g. in CCl4, add hexamethylenetetramine (I) 150 g. in 1 l. CCl4, filter the ketone-I complex after 3 h., keep 350 g. of this complex with 150 cc. 6 N HCl 1 h. at room temperature, and evaporate to dryness in
vacuo at room temperature to obtain 5-nitro-2-furyl aminomethyl ketone-HCl, 150
g. of which treated with 1 l. AcOH, 300 cc. Ac2O, and 85 g. NaOAc gives on
dilution with H2O 5-nitro-2-furyl acetamidomethyl ketone. Stirring this ketone 100 g. in MeOH 500 cc. and 40% CH2O 150 cc. with the addition of NaHCO3 5 g. gives 5-nitro-2-furyl 1-acetamido-2-hydroxyethyl ketone. Refluxing this latter compound 105 5 h. with (Me2CHO)3Al 180, and Me2CHOH 2
l., while N passes through and the Me2CO formed is distilled off, removing
the Me2CHOH in vacuo, heating the residue with 2 l. H2O at 100°, filtering, and cooling gives [dl]-ψ-1-(5-nitro-2-furyl)-2-acetamido-1,3-propanediol (II). Saturation of the aqueous filtrate with NaCl, extraction with
AcOEt, and evaporation gives a mixture of the dl-ψ and the dl-reg. compound,
which are separated by fractional crystallization Evaporating dl-ψ-II.HCl 50 g. in N
HCl 200 cc. after standing 24 h. gives dl-ψ-1-(5-nitro-2-furyl)-2-amino-1,3-propanediol-HCl (III). The insol. free base is obtained with NH3. The dl-reg.-II.HCl gives by the same method the reg. III.-HCl. Boiling dl-ψ-III 14.6 with d-tartaric acid 7.4 g. in MeOH 150 cc. 1 h. gives crystals (augmented by addnl. boiling with more MeOH), consisting of
l-ψ-III.HCl which gives with NaOH at pH 10 the free base. The MeOH filtrate of the reaction mixture of the tartrate gives on evaporation the d-ψ-III.HCl, which gives the base with NaOH. Heating l-ψ-III 4 g. with Cl2HCCO2Me 5 in MeOH 20 cc. 1 h., evaporation to dryness, and crystallization from
H2O gives 1-ψ-1-(5-nitro-2-furyl)-2-(dichloroacetoamido)-1,3-propanediol. The dl-compound is prepared by the analogous procedure. Shaking
dl-III base 5.4 g. with BzCl 4 in N NaOH 40 cc., and washing the crystals formed with dilute HCl, dilute NaHCO3 solution, and H2O gives dl-ψ-1-(5-nitro-2-furyl)-2-benzamido-1,3-propanediol. dl-III 2, Ac2O 4 g., and dry pyridine 2.5 cc., let stand 3 h. and then diluted with H2O give
the insol. dl-III triacetate. Heating dl-III 1.3 with Ac2O 3.5 g. 10 min.

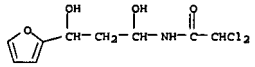
L8 ANSWER 124 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
at 70°, evapg. to dryness in vacuo, and recrystg. from MeOH gives dl-ψ-1-(5-nitro-2-furyl)-2-acetamido-3-acetoxy-1-propanol (IV). IV gives on standing with Ac2O and pyridine the tri-Ac compd. Shaking dl-III
with N KOH 60, Et2O 60 cc., and p-O2NC6H4COCl 2 g. gives insol. dl-ψ-1-(5-nitro-2-furyl)-2-(p-nitrobenzamido)-1,3-propanediol. dl-III 1 g. with furoyl chloride 1 in EtOAc 30 cc. at 0° gives (in the EtOAc) dl-ψ-1-(5-nitro-2-furyl)-2-furoylamido-1,3-propanediol. Moderately heating NaOMe 0.12 g. 30 min. with dl-III 4 and Me2C:CHCO2Et 5 in MeOH 50 cc., neutralizing with 2 cc. N HCl, removing the MeOH, and extg. the residue with C2H4Cl2 gives dl-ψ-1-(5-nitro-2-furyl)-2-(β, β-dimethylacrylylamino)-1,3-propanediol. Succinic anhydride 2 g. heated 30 min. with dl-III in H2O 40 cc. gives on standing dl-ψ-1-(5-nitro-2-furyl)-2-(β-carboxypropionylamino)-1,3-propanediol. From a soln. of I 75 g. in CCl4 100 cc. and 2-furyl bromomethyl ketone in 400 cc. CCl4 there crystallizes in 2 h. O.(CH2)3.CHCOCH2(CH2)6N4Br, 150 g. of which gives, after standing 45 min. with 800 cc. 6 N HCl and evapn. to dryness, O.(CH2)3.CHCOCH2NH2.HCl (V). Stirring V 50 with Ac2O 100, AcOH 400, and NaOAc 40 g. and dilg. with H2O gives 2-furyl acetamidomethyl ketone (VI). Heating VI 40 g. 30 min. with 40% CH2O 80 cc., NaHCO3, 2 g., and MeOH 350 cc. at 45° and pouring into 2 l. H2O gives 2-furyl 1-acetamido-2-hydroxyethyl ketone (VII). Refluxing VII with (Me2CHO)3Al and Me2CHOH 5 h. while the Me2CO formed is carried off by a stream of N, evapn. in vacuo, boiling the residue with H2O, and filtration gives dl-ψ-1-(2-furyl)-2-acetamido-1,3-propanediol (dl-VIII). From the mother liq. are obtained addnl. dl-ψ- and dl-reg.-compd. sepd. by fractionate crystn. from EtOH and H2O. In analogy
with the compds. described before are prepd. the di-Ac deriv. of VII, the dl- and l-ψ-1-(2-furyl)-2-amino-1,3-propanediol (IX), the N-COCHCl2 deriv. of l- and dl-IX, the tribenzoate of dl-IX. Keeping a mixt. of 5-methyl-2-furyl bromomethylketone-I complex, 175 g. with 1 l. 6 N HBr 45 min. at room temp. and evapg. to dryness gives O.CHMe.(CH2)2.CHCOCH2NH2.HBr, which with PhCH2COCl in pyridine at a temp. below 5° gives the phenylacetyl deriv. From this are prepd. 5-methyl-2-furyl 1-phenylacetamido-2-hydroxyethyl ketone and of 1-(5-methyl-2-furyl)-2-amino-1,3-propane diol (X), the N-COCH2Ph deriv., the N-MeOCH2CO deriv., the O,O,N-(PhCH2CO)2 (MeOCH2CO) deriv., the N-NCH2CO deriv., and the N-COCH(OH)Me deriv. of dl-ψ-X, and the N-3-pyridylcarbonyl deriv. of the dl-reg.-X. A series of 5-iodo analogs, with and without Bz and Ac substitutions, starting with the 5-iodo-2-furyl
bromomethyl-I complex are described.

ACCESSION NUMBER: 1951:55792 HCAPLUS
DOCUMENT NUMBER: 45:55792
ORIGINAL REFERENCE NO.: 45:9564b-i,9565a-d
TITLE: Furan compounds
INVENTOR(S): Long, Loren M.; Jenesel, Nickolas D.
PATENT ASSIGNEE(S): Parke, Davis & Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2547712		19510403	US 1949-83769	19490326

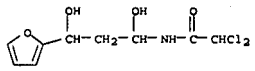
IT 793696-69-2, Acetamide, 2,2-dichloro-N-[2-(2-furyl)-2-hydroxy-1-(hydroxymethyl)ethyl]-

L8 ANSWER 124 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(stereoisomers)
RN 793696-69-2 HCAPLUS
CN Acetamide, 2,2-dichloro-N-[2-(2-furyl)-2-hydroxy-1-(hydroxymethyl)ethyl]- (5CI) (CA INDEX NAME)



L8 ANSWER 125 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB threo-1-(2-Furyl)-2-amino-1,3-propanediol (I) and some derivs. are prepared as intermediates for a synthesis of the nitrofuryl analog of chloramphenicol. PhCH(NH2)CH(OH)CO2H (12.6 g.), m. 194°, prepared according to Erlenmeyer [Ber. 25, 3445(1892)] in 42% yield, is converted with EtOH and HCl into 91% Et ester-HCl (II), m. 136-7°. Adding the free ester from 3.5 g. II in 100 cc. ether to 1.8 g. LiAlH4 in 75 cc. ether, refluxing the mixture 1.5 h., decomposing the excess LiAlH4 with 8 cc. H2O, washing the precipitate with ether, evaporating the ether solution, and treating the residue with alc. (CO2H)2 give 47% PhCH(OH)CH(NH2)CH2OH(III) oxalate, C10H14NO4, m. 217°, which, treated with the equivalent amount of Ba(OH)2, gives III, m. 86-7° (N-Bz derivative, prepared with BzCl and 20% NaOH, m. 165-6°). Adding 268 g. KOH in 1200 cc. absolute EtOH over a period of 70 min. to 460 g. freshly distilled 2-furaldehyde and 180 g. glycine in 800 cc. EtOH at 3° and keeping the mixture 24 h. below 10° and the filtered solution another 24 h. give RCH(OH)CH(N:CHR)CO2K (R = O.CH:CH.CH:C throughout the abstract) (IV), m. 151-2° (decomposition). Decomposing IV in 750 cc. H2O with 130 cc. AcOH with addition of 750 cc. EtOH gives 48% RCH(OH)CH(NH2)CO2H (V), m. 207-8°. Treating V with BzCl and alkali gives 2-phenyl-4-furfurylidene-5(4H)-oxazalone, m. 170°. Treating 51 g. V in 650 cc. EtOH with 146 cc. 10.4 N alc. HCl and 850 cc. EtOH 5 days at 20° and neutralizing the mixture with EtONa give 73% Et ester (VI), m. 77-8° (oxalate, m. 141°). Reducing 47.2 g. VI with LiAlH4 and treating the product with (CO2H)2 give 50% RCH(OH)CH(NH2)CH2OH (VII) oxalate (VIIa), m. 227-8°, which with the calculated amount of Ba(OH)2 gives VII, m. 62.5-3°. RCOCH2CO2Et, b12 135-9°, with PhN2Cl buffered with NaOAc, at 0-5°, gives 91% Et α-phenylazo-2-furoylacetate, m. 67-7.5°. Treating RCOCH2CO2Me, b8-9 120°, in 150 cc. AcOH at 5-8° with 21.5 g. NaNO2 in 30 cc. H2O, stirring the mixture 1.75 h., adding 500 cc. H2O, and extracting it with ether give 83% RCOC(:NOH)CO2Me (VIII), m. 125-5.5°; Et ester (IX), prepared in 59% yield, m. 133-5°. Treating 44.4 g. VIII in 160 cc. AcOH and 40 cc. Ac2O in the presence of 3.5 g. 5% Pd-charcoal with H at 2-3 atmospheric at 20°, evaporating the filtered solution in vacuo, and recrystg. the residue give 79% RCOCH(NHAc)CO2Me, m. 105-5.2°. Adding 12 g. LiAlH4 in 200 cc. dry ether to 10.6 g. IX over a period of 1 h. and refluxing the mixture 2 h. give 200 mg. VIIa, m. 226-7° (decomposition) (N-Bz derivative, long needles, m. 105-6°). Heating 9.05 g. VII 2 h. with Cl2CHCO2Me at 90-100° gives 52% N-Cl2CHCO derivative (X), m. 88.5-9°. Treating VII from 5.45 g. VIIa with 20 cc. Ac2O and 20 cc. C5H5N below 65°, keeping the mixture 11 h., heating it 2 h., and evaporating in vacuo give a light brown oil from which, on crystallization from EtOAc-(Me2CH)2O (1:20), 83.5% RCH(OAc)CH(NHAc)CH2OAc (XI), m. 92-2.5°, is obtained. Heating 2.68 g. X with 5 cc. Ac2O and 5 cc. C5H5N 1 h. at 100°, evaporating the

L8 ANSWER 125 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
mixt., and recrystg. the residue give 81% RCH(OAc)CH(NHCOCHCl2)CH2OAc (XII), m. 87.8-8.3°. Adding 8.5 g. XI in 19 cc. Ac2O to a cooled mixt. of 6 cc. concd. HNO3 and 22.5 cc. Ac2O below 25°, stirring the mixt. 0.5 h. at 40°, adding 20 cc. H2O with cooling, adjusting the mixt. with 190 cc. 20% Na3PO4 to pH 3.9, dilg. with 50 cc. H2O, heating 1 h. at 60°, extg. the cooled mixt. with AcOEt, and evapg. the washed (NaHCO3) AcOEt ext. give 5.8 g. of a brown oil, which, extd. with ether, gives 29% 1-(5-nitro-2-furyl)-2-acetamido-1,3-diacetoxypropane, bright yellow viscous oil, UV absorption ε3170A 9300 (assumed mol. wt. 328). A similar nitration of XII gives 66-9% 2-dichloroacetamido analog, ε3170A 8930 (assumed mol. wt. 397).
ACCESSION NUMBER: 1951:49881 HCAPLUS
DOCUMENT NUMBER: 45:49881
ORIGINAL REFERENCE NO.: 45:8504a-i
TITLE: The preparation of 1-(2-furyl)-2-amino-1,3-propanediol and derivatives
AUTHOR(S): Hayes, Kenyon; Gever, Gabriel
CORPORATE SOURCE: Eaton Labs., Norwich, NY
SOURCE: Journal of Organic Chemistry (1951), 16, 269-78
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 45:49881
IT 793696-69-2P, Acetamide, 2,2-dichloro-N-[2-(2-furyl)-2-hydroxy-1-(hydroxymethyl)ethyl]-
RL: PREP (Preparation)
(preparation of)
RN 793696-69-2 HCAPLUS
CN Acetamide, 2,2-dichloro-N-[2-(2-furyl)-2-hydroxy-1-(hydroxymethyl)ethyl]- (5CI) (CA INDEX NAME)



L8 ANSWER 126 OF 126 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 44, 584d. Me β-ethylacrylate b. 144-5°; Me β-propylacrylate b22 62-4°; iso-Pr isomer b22 60-2°. R2CHR1CH2CO2R were prepared by the following methods: (A) the amine in an equal volume of EtOH is mixed with MeCH:CHCO2Me(Et) and distilled after 14 days; (B) the amine and MeCH:CHCO2Me are refluxed 3 hrs.; (C) the addition of pyrrolidine to MeCH:CHCO2Me causes boiling; the mixture is distilled after standing overnight; (D) 1 mol. amine in an equal volume of EtOH is added to MeEtC:CH2CO2Me and distilled after 4 days; (E) this is the same as D but with 1.5 mols. amine. The following new R2CHR1CH2CO2R are reported: Yield,; R, R1, R2, Method, %, B.p., °C., mm.; Et, Me, NHBu, A, 80, 100, 17; Me, Me, NMe2, A, 79, 66, 17; Me, Me, NEt2, A, 57, 84, 18; Me, Me, NPr2, A, 40, 116-18, 15; Me, Me, NBu2, A, 29, 134-6, 15; Et, Me, NMeCH2Ph, B, 41, 156-8, 16; Me, Me, NC4H8, C, 89, 100-2, 23; Et, Me, N(CH2)4O, B, 42, 121-2, 12; Me, Et, NMe2, D, 50, 78-80, 18; E, 83; Et, Et, NMe2, E, 85, 88-90, 20; Me, Et, NC5H10, D, 65, 122-3, 21; E, 76; Et, Et, NC5H10, E, 73, 130-2, 21; Me, Pr, NMe2, E, 74, 90, 15; Et, Pr, NMe2, E, 83, 116-18, 24; Me, Pr, NC5H10, E, 69, 140-1, 22; Et, Pr, NC5H10, E, 49, 158-60, 30; Me, iso-Pr, NMe2, E, 69, 86-8, 24; Et, iso-Pr, NMe2, E, 72, 108-10, 25; Me, iso-Pr, NC5H10, E, 29, 130-3, 22; Et, iso-Pr, NC5H10, E, 26, 140-1, 17 The 3-amino-1,1-di(2-thienyl)-1-alkanols were prepared from 2-thienyllithium (prepared from BuLi) (I) and the appropriate β-amino ester, or from the Grignard reagent (II) from 2-bromothiophene and the ester (details of each preparation are given). R and R' are given for S.CH:CH.CH:CC(OH)CH2CHRR'. R = H;R' = NMe2, m. 136-7°, 72% (I) [oxalate, m. 170-1° (decomposition)]; R' = NEt2, m. 65°, 18% (II) [HCl salt, m. 196-7° (decomposition); methiodide, m. 193-4° (decomposition)]; R' = NC4H8, m. 118-19°, 73% (HCl salt, m. 196-7° (decomposition); methiodide, m. 179-80° (decomposition)]; R' = NC5H10, b0.04 176-80°, m. 70-2°, 66% (HCl salt, m. 198° (decomposition); methiodide, m. 126-7°]. R = Me;R' = NH2, m. 126-7°, 34% [acid oxalate, m. 151-2° (decomposition)]; R' = NHEt, b0.1 139-43°, m. 80-1° [acid oxalate, m. 204-5° (decomposition)]; R' = NHBu, m. 63-4°, 40% [acid oxalate, m. 183-4° (decomposition)]; R' = NMe2, m. 90-1°, 71% [HCl salt, m. 198-9° (decomposition); methiodide, m. 189°]; R' = NEt2, m. 75-6°, 79% (oxalate, m. 117-18°); R' = NPr2, m. 91-2°, 70% (oxalate, m. 100°); R' = NMeCH2Ph, m. 73-4°, 56% [oxalate, m. 143-4° (decomposition)]; R' = NC4H8, m. 88-9°, 77% [oxalate, m. 172-3° (decomposition)]; R' = NC5H10, b0.02 146-8°, m. 82-3° [oxalate, m. 166-7° (decomposition)]; R' = N(CH2)4O, m. 105-6°, 48% [oxalate, m. 134-5° (decomposition)]. R = Et, R' = NMe2, m. 83-4°, 73% (I) (oxalate, m. 170-1°); R = Pr, R' = NMe2, b0.05 145-7°, 43% (oxalate, m. 138-9° (decomposition)]; R = iso-Pr, R' = NMe2, m. 56-7°, 71% (oxalate, m. 125-6°). The above carbinols were dehydrated by refluxing with 30 cc. concentrated HCl and 100 cc. AcOH 20 min.,

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in certain cases warming on the steam bath was satisfactory. The following 3-amino-1,1-di(2-thienyl)-1-alkenes, (S.CH:CH.CH:C)2C:CHCHRR', were prepd. (the figures in brackets are the m.p. of the HCl salts). R = H;R' = NMe2, b0.05 91-4° [144-5°]; R' = NEt2 [116-17°]; R' = NC4H8 [102-3°]; R' = NC5H10, b0.05 143° [171-3° (decompn.)]. R = Me;R' = NH2 [174-5° (decompn.)]; R' = NHEt, b0.03 112-14° [134-5°]; R' = NHBu, b0.04 122-4° [123-4°]; R' = NMe2, b0.05 123-5° [169-70°]; R' = NEt2, b0.03 122-8° [152-3°]; R' = NPr2, b0.01 119-21° [112-15°]; R' = NMeCH2Ph, b0.01 146-8° [160-1° (decompn.)]; R' = NC4H8, b0.1 132-5° [167-9°]; R' = NC5H10, b0.05 132-6° [188-9°]; R' = N(CH2)4O, b0.05 130-6° [181-2°]. R = Et, R' = NMe2, b0.03 110-12° [138-9°]; R = Pr, R' = NMe2, b0.03 116-18° [158-9°]; R = iso-Pr, R' = NMe2, b0.03 107-9° (H oxalate, m. 159-60° (decompn.)]. Methiodides: 3-diethylamino-1,1-di(2-thienyl)-1-propene, m. 174-5° (decompn.); 3-(1-pyrrolidyl) analog, m. 186° (decompn.); 3-(1-piperidyl) analog, m. 193-4° (decompn.); 3-dimethylamino-1,1-di(2-thienyl)-1-butene, decomp. from 130°.
ACCESSION NUMBER: 1950:40768 HCAPLUS
DOCUMENT NUMBER: 44:40768
ORIGINAL REFERENCE NO.: 44:7825d-i,7826a-f
TITLE: Aminoalkyl tertiary carbinols and derived products. II. 3-Amino-1,1-di(2-thienyl)alkan-1-ols and -1-alkenes
AUTHOR(S): Adamson, D. W.
CORPORATE SOURCE: Wellcome Research Labs., Beckenham, UK
SOURCE: Journal of the Chemical Society (1950) 885-90
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 854462-96-7P, 1-Butanol, 3-butylamino-1,1-di-2-thienyl-
854464-57-6P, 1-Butanol, 3-ethylamino-1,1-di-2-thienyl-
855280-67-0P, 1-Butanol, 3-amino-1,1-di-2-thienyl-
855280-68-1P, 1-Butanol, 3-amino-1,1-di-2-thienyl-, oxalate (salt)
RL: PREP (Preparation)
(preparation of)
RN 854462-96-7 HCAPLUS
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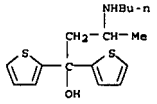

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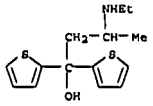

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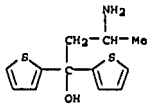

RN 855280-68-1 HCAPLUS
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CM 1

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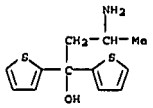

CM 2

CRN 144-62-7
CMF C2 H2 O4

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